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A TRANSIENT PERFORMANCE METHOD
FOR CO₂ REMOVAL WITH
REGENERABLE ADSORBENTS

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October 1972

Prepared Under
Contract No. NAS 1-8559

by

AIRESEARCH MANUFACTURING COMPANY
Los Angeles, California

for

National Aeronautics and Space Administration
Langley Research Center
Hampton, Virginia

A TRANSIENT PERFORMANCE METHOD FOR CO₂ REMOVAL WITH REGENERABLE ADSORBENTS

Prepared by
K.C. Hwang

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FOREWORD

Part I of this report describes a computer program (S9960) which can be used to predict the transient performance of vacuum-desorbed sorbent beds for CO₂ or water removal, and composite beds of two sorbents for simultaneous humidity control and CO₂ removal. The program was written primarily for silica gel and molecular-sieve inorganic sorbents, but can be used for a variety of adsorbent materials.

The initial development of the computer program was started under the Apollo Applications Program, Contract NAS9-3541, NASA Manned Spacecraft Center. Further improvements were made through the application of AiResearch R & D funds, and under Contract NASI-8559 from the NASA Langley Research Center which also funded the acquisition of additional basic adsorption data.

The content of Part I is as follows: Section 1 presents a general description of the program; Section 2 describes the technical details of the program; Section 3 describes program usage; and Section 4 presents an example of program usage; Subroutine documentation is given in Section 5, together with a complete listing of the program.

Part II of this report describes a computer program (MAIN4B) which can be used to predict performance for multiple-bed CO₂-removal sorbent systems. This program is an expanded version of the composite-sorbent-bed program, S9960, described in Part I.

The primary improvement included in MAIN4B is that the poisoning effect of water coadsorbed by the CO₂-removal bed is taken into account in predicting the CO₂ adsorption performance of the bed. The program also estimates coadsorption of oxygen, nitrogen, and subsequent overboard losses. The system simulation capabilities have been expanded to allow consideration of

- 2-bed vacuum-dump,
- 4-bed H₂O-save/CO₂-dump, and
- 4-bed H₂O-CO₂-save type systems.
- Beds may be thermally conditioned by heat-transport fluid passages within the bed, or by internal electrical heaters.

Although certain features of MAIN4B are completely new, or are considerably different from those incorporated in program S9960, much of the background material presented in Part I is used in the new program. Part II presents only material unique to MAIN4B. The complete documentation of the new program, for those interested in the techniques used in the program, or for those desiring to modify the program set, includes both Part I and Part II.

Nomenclature used in this report is presented at the beginning of each part. The content of Part II is as follows. Section 1 provides a general description of the program; Section 2 technically describes new features of MAIN4B that make it different than S9960; Section 3 describes input data for



FOREWORD (Cont)

program execution; and Section 4 presents two example runs with the program. Two appendixes furnish subprogram documentation (Appendix A) and a complete listing of the program (Appendix B).

Dr. K.C. Hwang of AiResearch, developed the computer programs described in this report, and also authored the report.

Mr. Rex Martin of NASA Langley Research Center was the technical monitor of Contract NASI-8559 during the development of these computer programs.



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PART I

COMPOSITE BED PROGRAM (S9960)

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NOMENCLATURE

<u>FORTRAN</u>	<u>Algebraic</u>	<u>Description</u>
A	$\left(\frac{f \cdot \rho_g \cdot u_q}{P \cdot M_g} \right)$	Quantity $\left(\frac{f \cdot \rho_g \cdot u_q}{P \cdot M_g} \right)$ appearing in Equation (2-35), (1b-mole)/(hr)(sq ft)(mm Hg)
ADT		Temporary storage for DT, hr
ADT2		Temporary storage for DT, hr
ABED	A	Cross-sectional area of adsorbent bed, sq ft
AGS,ASG	a_{sg}	External surface area of sorbent, sq ft/(cu ft of bed)
AGX,AXG	a_{xg}	Primary heat transfer area between heat exchanger and gas stream, sq ft/cu ft of sorbent bed
ASX,AXS	a_{xs}	Primary heat transfer area between heat exchanger and sorbent, identical to a_{xg}
AVC	a_{vc}	Primary heat transfer area for coolant, sq ft/(cu ft of coolant volume)
AVLD		Average loading at each axial node, (1b-sorbate)/(1b- sorbent)
AVH2OP		Average poisoning rate of molecular sieves by H_2O , (1b- H_2O)/hr
AVMSLD		Average CO_2 -loading of all active molecular sieve sor- bents, 1b- CO_2 /(1b-molecular sieves)
AVPH2O		Average outlet P_{H_2O} , mm Hg
AVRCO2		Average CO_2 adsorption or desorption rate, 1b- CO_2 /hr
AVRH2O		Average H_2O adsorption or desorption rate, 1b- H_2O /hr
AVSGLD		Average H_2O -loading of desiccant sorbents, 1b- H_2O /(1b- desiccant)
AVX	a_{vx}	Primary heat transfer area for heat exchanger, sq ft plate area/(cu ft of metal)
B		Temporary variable used in simultaneous solution of a system of finite difference equations. See Equations (2-41) and (2-42)



<u>FORTRAN</u>	<u>Algebraic</u>	<u>Description</u>
C	C	Molal density of gas mixture, lb moles/(cu ft)
CPC	c_{pc}	Heat capacity of coolant, Btu/({}^{\circ}F)(lb)
CPG	c_{pg}	Heat capacity of gas mixture, Btu/({}^{\circ}F)(lb)
CPS	c_{ps}	Sorbent specific heat, Btu/(lb)({}^{\circ}F)
CPX	c_{px}	Heat capacity of heat exchanger metal, Btu/({}^{\circ}F)(lb)
CPI		{ Coefficients in equation
CP2		$CP3 \cdot \left(p_{ks,t+\Delta t} - X_k P_{t+\Delta t} \right) = CPI + CP2 \cdot P_{t+\Delta t}$
CR1		{ Coefficients in following equation which is merely another form of Equation (2-28).
CR2		
CR3		$CR1 \cdot \frac{W_{k,M,(t+\Delta t)} - W_{k,M,t}}{(\Delta t)} = CR2 \cdot (W_{k,(M-1),(t+\Delta t)} - W_{k,M,(t+\Delta t)}) + CR3 \cdot (W_{k,M,(t+\Delta t)} - W_{k,(M+1),(t+\Delta t)})$
CSI		{ Coefficients in equation
CS2		$T_{s,(t+\Delta t)} - T_{s,t} = DS + CSI \cdot P_{(t+\Delta t)} - CS2 \cdot p_{ks,(t+\Delta t)}$
CYCLE		Cycle time per one adsorption or one desorption half-cycle, hr
C1		{ Coefficients in equation
C2		$C1 \cdot W_{(t+\Delta t),(M-1)} + C2 \cdot W_{(t+\Delta t),M} + C3 \cdot W_{(t+\Delta t),(M+1)} = DI$
C3		
CIP		{ Coefficients in equation
C2P		$CIP \cdot P_{(t+\Delta t),(N-1)} + C2P \cdot P_{(t+\Delta t),N} + C3P \cdot P_{(t+\Delta t),(N+1)} = DIP$
C3P		
DH	ΔH	Heat of adsorption at each node Btu/(lb adsorbed)
DIF	D_k	Mass diffusivity of component k through the interior of sorbent, sq ft/hr



<u>FORTRAN</u>	<u>Algebraic</u>	<u>Description</u>
DPC ϕ 2C		Cabin CO ₂ partial pressure increase in one time increment, mm Hg
DS		See CSI
DT ϕ		Time increment of previous computation step, hr
DT	Δt	Time increment, hr
DTMAX		Maximum allowable time step size, usually 0.01 hr for isothermal analysis and 0.005 hr for nonisothermal analysis
DVS		Size of interior sorbent volume elements, (cu ft)
DVS1		Size of sorbent volume elements at surface and center of spherical pellets, DVS1 = 1/2 DVS, (cu ft)
DX		Axial node dimension, ft
DI		See CI
DIP		See CIP
D2		Coefficient in equation $W_{ks} = Q + D2 \cdot P_{(t+\Delta t)}$
D9		DT in single precision, hr
F	F	Factor defined by Equation (2-17), a function of pressure
FR		Molal flow rates of CO ₂ and H ₂ O, during desorption, FR(1,N) is CO ₂ rate, FR(2,N) is H ₂ O rate, lb-mole/hr
G		Mass flux = $u_g \cdot \rho_g$, lb/(hr)(sq ft void area)
GK	K _g	Mass transfer coefficient between bulk stream and the surface of adsorbent. Surface kinetic rate can be incorporated in this coefficient, lb-moles/(hr)(sq ft) (mm Hg)
GMR	G _t	Total mass flow rate, lb/(hr)
GMW	M _g	Average molecular weight of process gas
HCX, HXC	h _{xc}	Heat transfer coefficient between heat exchanger primary plate and coolant, Btu/(sq ft)(°F)(hr)



<u>FORTRAN</u>	<u>Algebraic</u>	<u>Description</u>
HGS,HSG	h_{sg}	Heat transfer coefficient between sorbent and gas, based on a_{sg} , Btu/(sq ft)(°F)(hr)
HSX,HXS	h_{xs}	Effective heat transfer coefficient between heat exchanger primary plate and sorbent, Btu/(sq ft)(°F)(hr).
\dot{M}_{sg}		Molar rate of mass transfer into bulk gas stream/unit bed volume, lb-moles per (cu ft of bed)(hr); see Equation (2-15)
M_s		Interior node corresponding to the surface of pellet
NBC ϕ UT		Integer control variable, if NBC ϕ UT = 2, the outlet manifold pressure is specified as a function of time; NBC ϕ UT = 1, the manifold pressure is computed from vacuum duct resistance
NCYCLE		Number of complete adsorption-desorption cycles from beginning of run
NCYCLT		Total number of complete adsorption-desorption cycle calculations desired
NDR4		Integer denoting total number of radial sorbent pellet nodes (interior nodes)
NDTC ϕ N		If = 1, internal Δt calculations. If = 2, fixed Δt 's in program will be used.
NDXM		Integer denoting total number of molecular sieve nodes
NDXMAC		Integer denoting number of active molecular sieve nodes, i.e., (NDXM-NDXMAX) represents the number of molecular sieve nodes which have been inactivated by water poisoning
NDXI		Integer denoting total number of axial nodes
N ϕ G		Node to which coolant is added
NPR		Number of time steps elapsed since last printout
NPRINT		Integer control variable which determines the frequency of printout occurrence; e.g., if NPRINT = 5, printout occurs after every five time steps
NPSET		Integers which denote the nodes to which tabulated vacuum history is applicable



<u>FORTRAN</u>	<u>Algebraic</u>	<u>Description</u>
NSTART		Integer denoting the cycle from which on bed performance will be printed at frequency specified by NPRINT
NTEMP		Integer control variable; If NTEMP = 0, the energy equations will be ignored and bed temperatures set equal to T268; If NTEMP \neq 0, heat balances will be performed
PA	P	System total pressure during adsorption, mm Hg
PC ϕ 2C		CO_2 partial pressure in cabin, mm Hg
PC ϕ 2I		CO_2 partial pressure at adsorption bed inlet, mm Hg
PCI	$\left. \begin{array}{l} \text{Coefficients in equation for desorption pressure} \\ \\ \frac{P_{(t+\Delta t),N} - P_{t,N}}{(\Delta t)} = PCI \cdot \frac{P_{(t+\Delta t),(N-1)} - 2P_{(t+\Delta t),N} + P_{(t+\Delta t),(N+1)}}{(\Delta x)^2} \\ \\ + PC2 \cdot \frac{P_{(t+\Delta t),(N+1)} - P_{(t+\Delta t),(N-1)}}{2(\Delta x)} \\ \\ + PC3 \cdot [p_{ks}(t+\Delta t) - X_k P_{(t+\Delta t)}] \end{array} \right\}$	
PC2		
PC3		
PH2 ϕ I		Inlet H_2O partial pressure, mm Hg
PK	p_k	$P \cdot X_k$; partial pressure of component k in bulk gas stream, mm Hg
P ϕ UT		10 tabulated desorption outlet pressures at TIMET, mm Hg
PT	P	Total pressure in bulk gas stream, mm Hg
P1	$\left. \begin{array}{l} \text{Coefficients in equation} \\ \\ p_{ks}(t+\Delta t) = P1 + P2 \cdot (w_{k,s(t+\Delta t)} - w_{k,s,t}) + P3 \cdot P \end{array} \right\}$	
P2		
P3		
Q		Temporary variable like B. See Equations (2-43) and (2-44)
r		Radial distance from center of sphere, ft
r _M		r at interior node M, ft



<u>FORTRAN</u>	<u>Algebraic</u>	<u>Description</u>
	r_s	Average particle radius found from ρ_{sb} and a_{sg} , ft
$RC\phi 2C$		Rate of CO_2 generation in cabin, 1b CO_2 per hr
$RGAS$	R	Gas constant, 554. (mm Hg) (cu ft)/(1b-mole) (°R)
$RH\phi C$	ρ_c	Coolant density, 1b/(cu ft)
$RH\phi G$	ρ_g	Gas density, 1b/(cu ft)
$RH\phi S$	ρ_s	Sorbent density, 1b/(cu ft particle)
$RH\phi SB$	ρ_{sb}	Sorbent bulk density, 1b/(cu ft bed volume)
$RH\phi X$	ρ_x	HX core metal density, 1b/(cu ft)
RS	r_s	Average particle radius found from ρ_{sb} and a_{sg} , ft
RSI		Radius of spherical surface separating two interior sorbent volume elements, ft
SK	k_s	Effective thermal conductivity of sorbent bed, Btu/(hr) (sq ft) (°F/ft)
$SUMPTM$		Quantity $\sum_t P_{H_2O, \text{outlet}} \cdot (\Delta t)$, (mm) (hr) t = zero
TC	T_c	Coolant temperature, °F
$TC1$		Coolant temperature at time, $t-\Delta t$
$TC2$		Coolant temperature at time, $t-2\Delta t$
TG	T_g	Gas temperature, °F
TGI	T_{gi}	Inlet gas temperature for adsorption cycle, °F



<u>FORTRAN</u>	<u>Algebraic</u>	<u>Description</u>
TI		Maximum temperature change allowable per time increment in selecting Δt , $^{\circ}\text{F}$
TIME	t	Time from beginning of each adsorption or desorption period, hr
TIMEM		Time above in minutes.
TIMET		10 times at which P_{OUT} are tabulated, hr
TKX	k_x	Thermal conductivity of heat exchanger core metal, Btu/(hr) (sq ft) ($^{\circ}\text{F}/\text{ft}$)
$T_0TC\phi 2$		Total amount of CO_2 adsorbed since beginning of adsorption period, lb
$T_0TH2\phi$		Total amount of H_2O adsorbed since beginning of adsorption period, lb
TS	T_s	Sorbent temperature, $^{\circ}\text{F}$
TS1		Sorbent temperature at time $t-(\Delta t)$, $^{\circ}\text{F}$
TS2		Sorbent temperature at time $t-2(\Delta t)$, $^{\circ}\text{F}$
TX	T_x	Heat exchanger core metal temperature, $^{\circ}\text{F}$
TX1		Heat exchanger core metal temperature at time $t-(\Delta t)$, $^{\circ}\text{F}$
TX2		Heat exchanger core metal temperature at time $t-2(\Delta t)$, $^{\circ}\text{F}$
T268	T_{268}	Inlet glycol temperature, $^{\circ}\text{F}$
UC	u_c	Coolant velocity, ft/hr
UG	u_g	Interstitial gas velocity, i.e., true gas velocity, ft/hr
VMS		Total bulk volume of molecular sieve sorbents, cu ft



<u>FORTRAN</u>	<u>Algebraic</u>	<u>Description</u>
ϕ_{IDF}	f	Void fraction of bed
ϕ_{LCAB}		Cabin volume for atmosphere, cu ft; use $VOLCAB = 10^{20}$, for constant PCO ₂ C
VS		Volume of a single sorbent pellet, cu ft
VSG		Total bulk volume of desiccants, cu ft
W	w_k	Local loading of component k in sorbent, lb sorbate k/lb sorbent
	$w_d(P)$	A function of pressure which represents the capacity of vacuum duct at duct inlet pressure of P mm, lb/hr
WI		Maximum loading change allowable per time increment in selecting Δt , lb/lb
WM	M_k	Molecular weight of component K. K = 1 and 2
WS		Temporary storage variable for W
WTACMS		Total weight of active molecular sieve sorbents, lb
WTMS		Total weight of molecular sieve sorbents, lb
WTSG		Total weight of desiccants, lb
X	x_k	Mole fraction of component k in gas stream k=1 refers to CO ₂ in molecular sieve bed gas stream, and K=2 refers to H ₂ O in desiccant bed gas stream
	x	Distance from molecular sieve bed end, ft
	y	Any of bed properties, T _s , T _x , w _k , T _c , T _g

Subscripts

- b Bulk
c Coolant
g Gas stream



Subscripts

i Inlet
k Component k
M Radial location index for sorbent interior nodes
N Axial location index
s Surface of sorbent
s Sorbent
t At time t
v Volume
x Heat exchanger

Superscripts

* Equilibrium quantity



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SECTION I

GENERAL DESCRIPTION

INTRODUCTION

The present computer program package for the Univac 1108 computer, S9960 through S9999, was developed to predict the transient performance of a composite molecular sieve/desiccant bed for CO_2 removal, which may be operated under either adiabatic or thermal swing conditions. The program is limited to cases where sorbents are regenerated by dumping to vacuum.

An attempt was made to solve the actual physical problem as rigorously and generally as was feasible. Thus, transient pressure variations during a desorption cycle are not arbitrarily set, but are calculated from the AiResearch test data (as shown here) for the flow of nitrogen gas under low pressures through a 5/8-in.-ID molecular sieve bed. For program flexibility, most of the physical properties and transfer rate constants are allowed to vary as a function of the bed location. Such a flexibility allows for the use of different heat exchanger configurations and different modes of operation for the molecular sieve bed and the desiccant bed.

The program does not assume any specific heat exchanger configuration for thermal control and is, therefore, applicable to cases where sorbent temperatures are regulated by cooling coils, plate-fin heat exchangers or process gas streams alone, and so forth. However, to implement this general approach, heat transfer coefficients for heat balance calculations are not computed in the program but must be supplied as input data.

The mass-transfer equations are written to permit both intraparticle diffusion and surface resistance. Either process can be made to control by proper choice of the appropriate coefficients in the input.

To minimize the running time of the program, an implicit scheme as proposed by Hwang (Reference 1) was employed for transient mass transfer calculation and a method somewhat similar to the one proposed by DuFort and Frankel (Reference 2) for solving a diffusion equation was used to handle the coupling terms of the energy equations for the transient temperature changes of the metal parts, the sorbent, and the coolant. The program, therefore, permits the use of allowable large time increments for accuracy considerations.

Program S9960 performs adsorption and desorption calculations for a specified number of complete cycles. Programs S9950 and S9951 perform adsorption and desorption calculations, respectively, for one-half cycle only. With all physical properties and operation parameters inputted through two block data subprograms, the programs will compute and print out temperature and bed loading changes as a function of time. Average bed loadings and average rates of adsorption and desorption are also printed.



MATHEMATICAL MODEL

An example of a sorbent bed for CO_2 -removal is depicted in Figure I-1. The unit shows the detail of construction. It is basically a plate-fin gas-liquid heat exchanger with sorbents packed between the fins in the gas side.

In the present program, bed properties are assumed to vary only in the direction of the process gas flow, and that coolant is either parallel or counter-current but cannot be cross flow to the gas flow. Electric analogs of the heat transfer in the idealized sorbent bed during adsorption and desorption are shown in Figures I-2 and I-3. Figures I-4 and I-5 show electric analogs for mass transfer processes involved in the bed during the adsorption and desorption periods, respectively. Although a plate-fin heat exchanger is shown in Figure I-1, the analogs of Figures I-2 through I-5 should still be valid for cases where other means of thermal control are used.

The resistances to thermal transfer in Figures I-2 and I-3 can be easily estimated from thermal conductivities of materials used. The mass transfer resistances in Figures I-4 and I-5, however, must be determined from actual bed performance data.

Although heat and mass transfer processes are shown separately, a coupling does exist between the two. In Figure I-2 the "I's" represent the rates of heat generation at various nodes due to various rates of sorbate adsorption by these nodes, which are the mass transfer rates across the sorbent surface resistances shown in Figure I-4. Similarly the "I's" in Figure I-3 are coupled with the mass transfer rates in Figure I-5.

PROGRAM CAPABILITIES

Uses

Program S9950 predicts the performance of a single adsorption period. It is used for analyzing a breakthrough curve that is obtained from a known initial bed conditions, such as an adsorption run which is made immediately after a bakeout. By a few trial-and-error runs of this program, the mass transfer coefficient and mass diffusivity for the test system can be found.

Program S9951 predicts the performance of a single vacuum desorption period. It is used to determine mass transport properties of a sorbent-sorbate system if a desorption run started from known initial conditions is available.

Program S9960 is designed to predict the performance of a cyclically regenerated adsorption-desorption system comprising a desiccant and a CO_2 sorbent bed. Although the program is not designed for bed-sizing, no more than three trials are usually required to zero in on a correct design to meet



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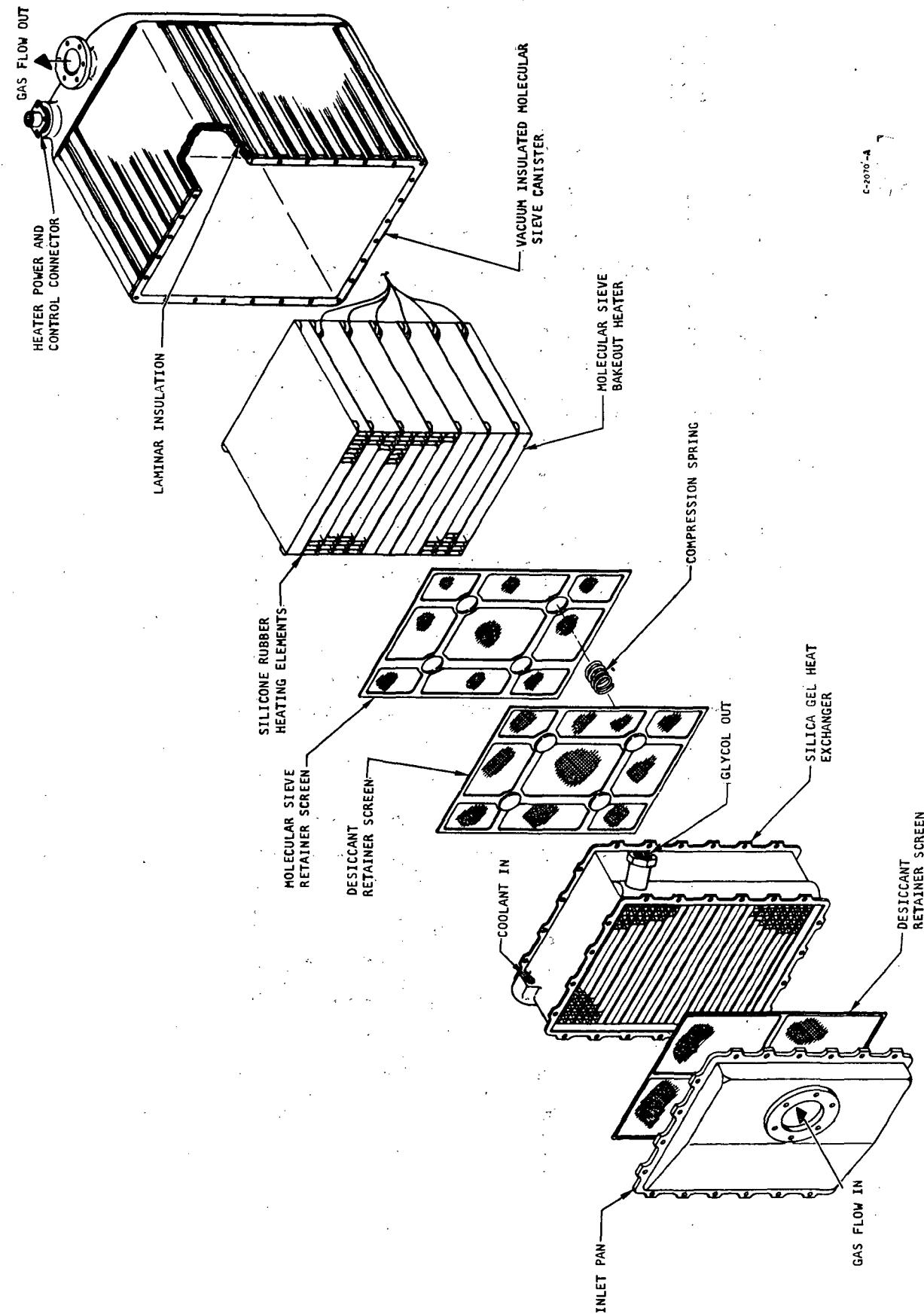


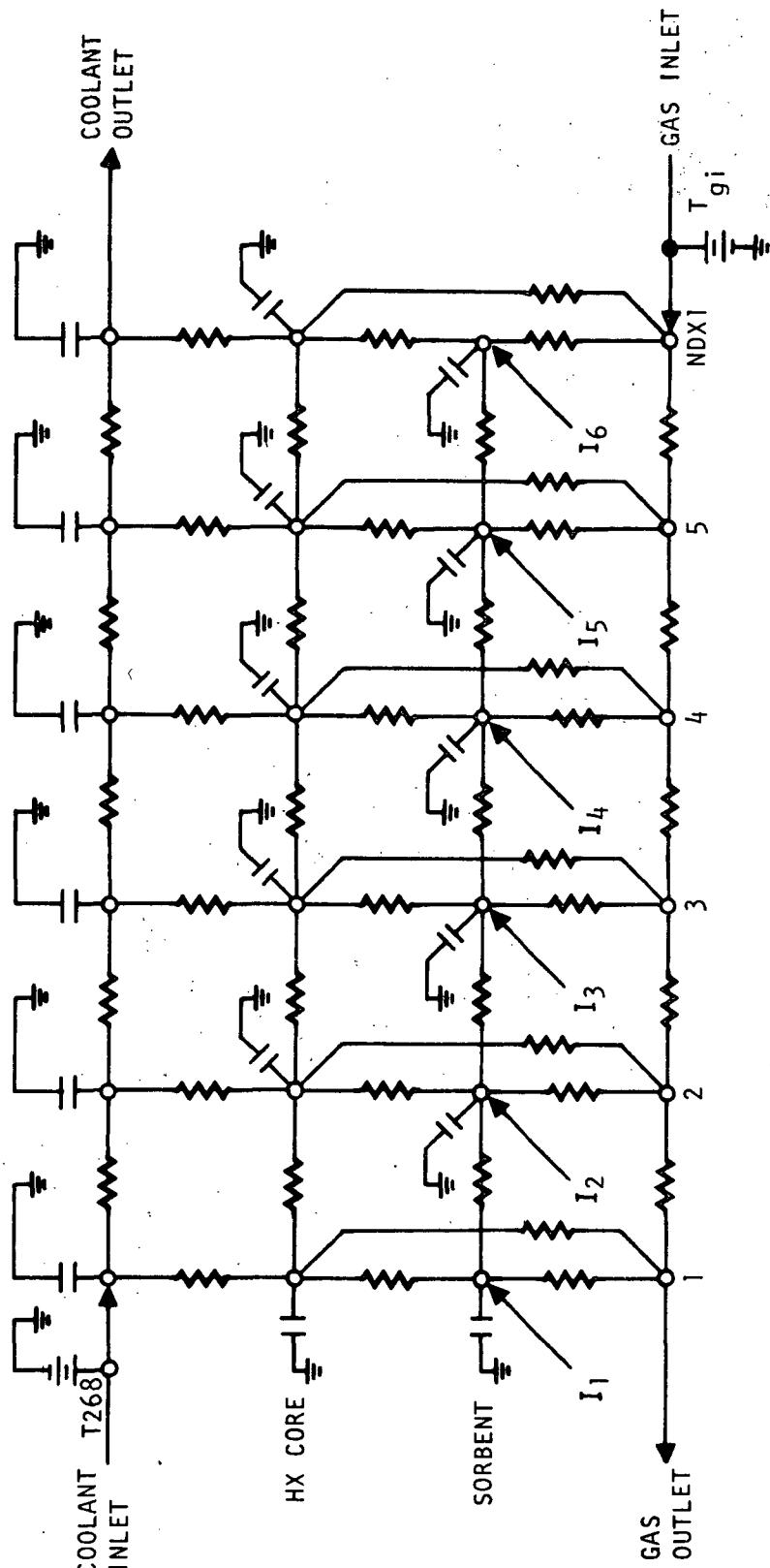
Figure I-1. Typical Adsorbent Canister



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Figure 1-2. Thermal Network for Sorbent Bed During Adsorption

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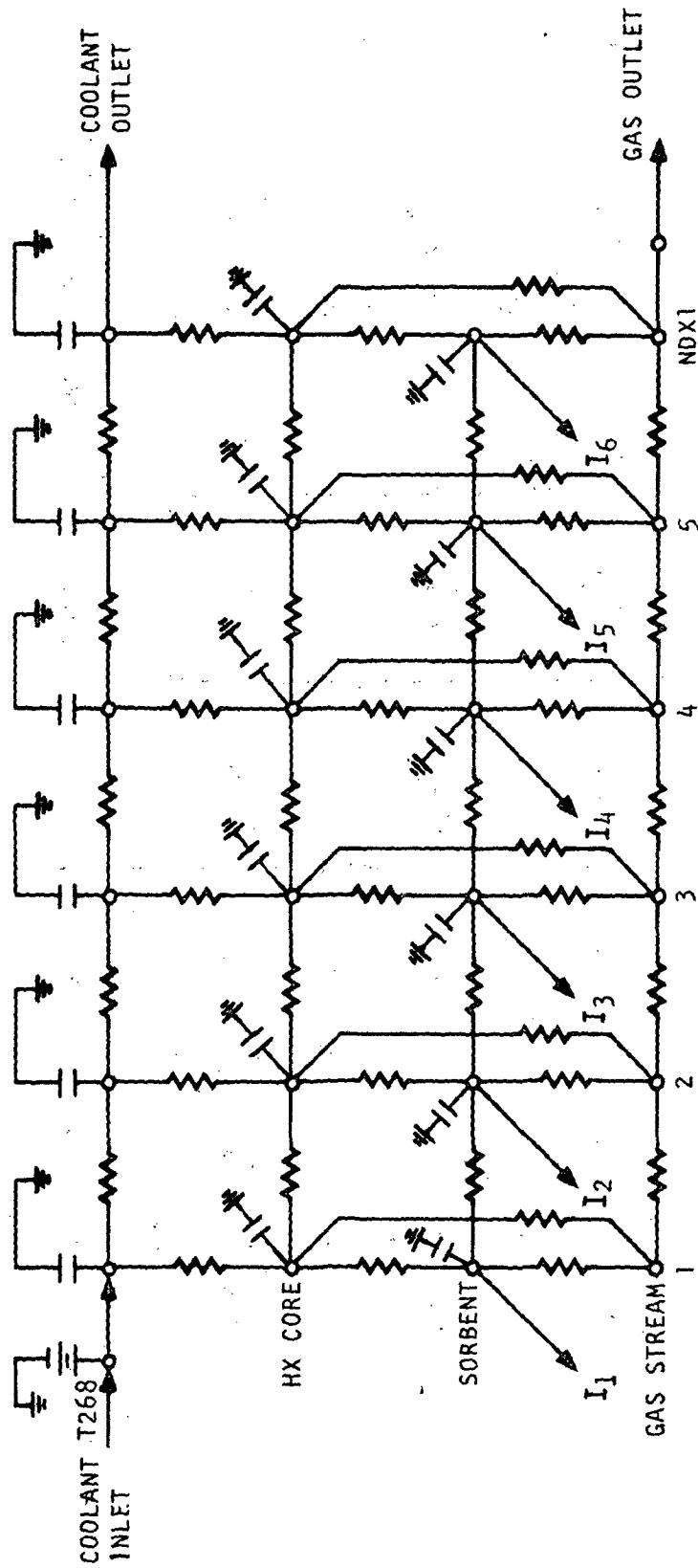
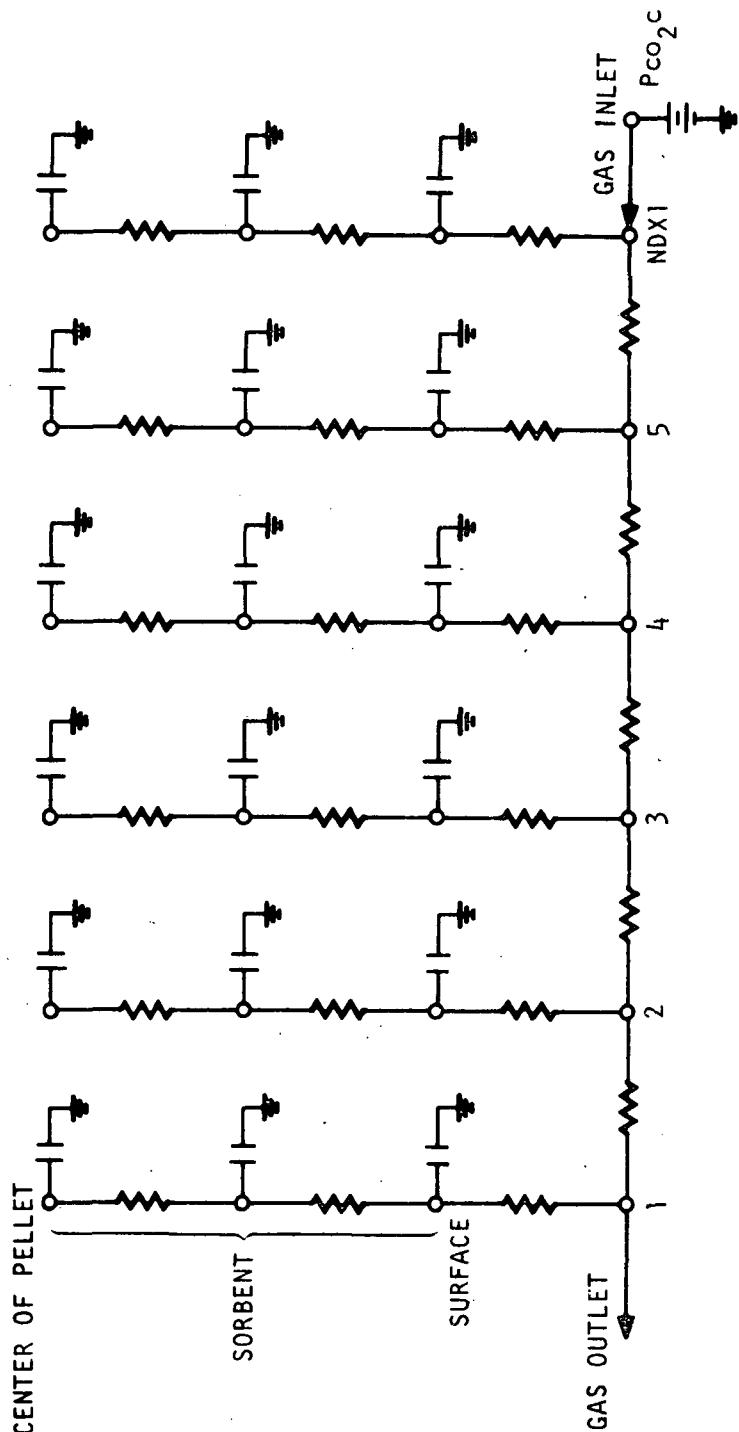


Figure 1-3. Thermal Network for Sorbent Bed During Desorption

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Figure 1-4. Mass Transfer Model for Sorbent Bed During Adsorption

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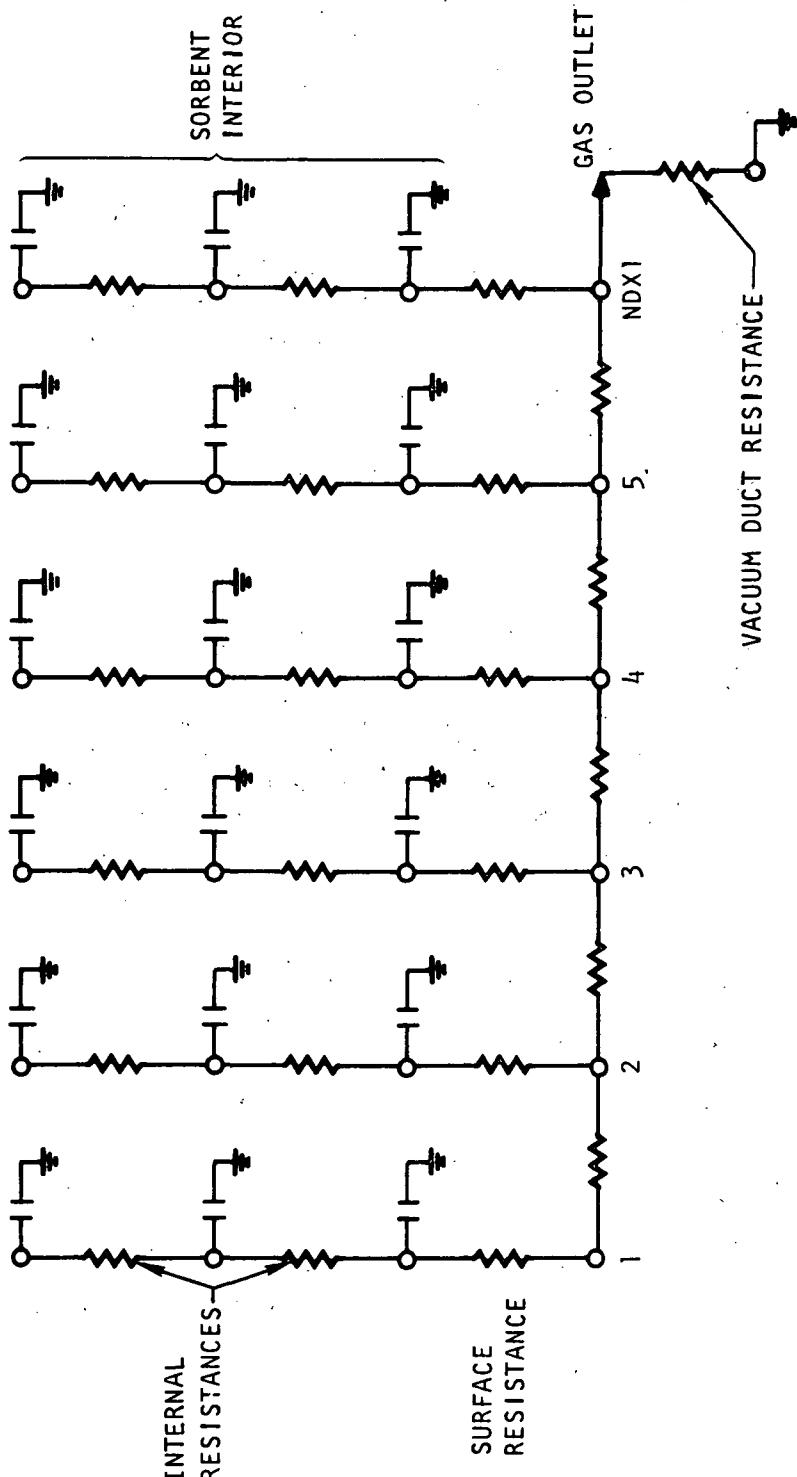


Figure 1-5. Mass Transfer Model for Sorbent Bed During Vacuum Desorption



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specified performance requirements, if operating parameters are given. To optimize an entire vacuum-dump CO_2 -removal system, the program can be used to generate curves showing the effects on total system weight of various parameters such as the process gas flow rate, bed size, coolant rate, and so forth. An optimum system can be easily found from that set of curves.

The program permits use of variable bed properties along the flow passage, and therefore, can be used for radial beds or beds of any arbitrary geometric configurations.

Input

The input to S9960 is by means of two BLOCK DATA subprograms, one for the adsorption period and the other for the desorption period computations. When running S9950 or S9951, only one pertinent BLOCK DATA subprogram is required.

In addition to the two block data subprograms, subprogram S9992 (PKEQ), which computes equilibrium vapor pressures of H_2O over the desiccant and CO_2 over the molecular sieve sorbent employed in the system, must be compiled with each run.

Output

Output from S9960 is the printed page. The output gives bed sizes, temperatures, sorbate loadings, partial pressures of CO_2 and H_2O during adsorption, total pressures during desorption, and average adsorption and desorption rates. Except at the end of each half cycle, the printout of bed properties will not appear until a number of adsorption-desorption cycles as specified by the input has been performed. The frequency of printout is also specified by the input.

Program Options

Various options available are summarized as follows:

- Use of S9950 for one half-cycle adsorption calculations
- Use of S9951 for one half-cycle desorption calculations
- Isothermal operation with the bed temperature specified
- Non-isothermal operation with the inlet coolant temperature specified
- Bed outlet pressure history during desorption inputted
- Bed outlet pressures computed from vacuum duct characteristics



- Bed cross-sectional areas vary in the axial direction
- Allowance of some inert nodes in the bed to simulate the case of partially poisoned bed
- Multi-outlet desorption with pressure history specified at up to three axial nodes

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SECTION 2
TECHNICAL DESCRIPTION

GENERAL ASSUMPTIONS

In addition to some minor approximations that are presented under the derivation of equations, the following general assumptions were made in deriving the differential equations which were employed in the present program.

<u>Assumption</u>	<u>Description</u>
A	Temperature gradient in the pellet interior is negligible.
B	Adsorption occurs by the diffusion of an adsorbate through the stagnant surface film at the exterior surface of an adsorbent particle condensing at the surface and then diffusion into the interior of the particle. Desorption occurs in a reverse fashion.
C	Adsorbent pellets can be represented by spherical particles for mass transfer calculations.
D	Heats of adsorption and desorption do not depend on temperature or concentration.
E	In the adsorption half cycle, the total flow rate and density of the gas stream are constant.
F	Bed properties do not vary in the direction perpendicular to the direction of the gas flow.

DIFFERENTIAL MODEL

Only those equations that are not obvious will be given their derivations here. The equations which are assumed to be obvious or easily derived by the reader are listed with appropriate boundary conditions without proof. Initial conditions of the equations are omitted, since they should be apparent.

Diffusion Equation for Interior of Sorbent Pellet

$$\frac{\partial w_k}{\partial t} = \frac{D_k}{\rho_s} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial w_k}{\partial r} \right) \quad (2-1)$$

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Boundary conditions are

$$\frac{\partial w_k}{\partial r} = 0 \text{ at } r = 0 \quad (2-2)$$

$$-\rho_s D_k \frac{\partial w_k}{\partial r} = M_k K_g \left(p_{k_s} - P + X_k \right) \text{ at } r = r_s \quad (2-3)$$

Energy Equation for Gas Stream

As the thermal capacitance of the gas in the void space of a sorbent bed is negligible compared with that of the sorbent bed or the heat exchanger core, a quasi-steady-state assumption can be made and the following is obtained, as energy equation for the gas stream,

$$\frac{dT_g}{dx} = \frac{1}{f \cdot \rho_g \cdot C_{pg} \cdot u_g} \left[a_{sg} \cdot h_{sg} \cdot (T_s - T_g) + a_{xg} \cdot h_{xg} \cdot (T_x - T_g) \right] \quad (2-4)$$

Equation (2-4) is subject to a boundary condition

$$T_g = T_{gi} \text{ at } x = x_0 \text{ (i.e., process gas inlet)} \quad (2-5)$$

for the adsorption half cycle, while for the desorption half cycle, the condition to be satisfied is

$$T_g = T_s \text{ at } x = 0 \quad (2-6)$$

Energy Equation for Sorbent

$$\begin{aligned} \frac{\partial T_s}{\partial t} &= \frac{\partial}{C_{ps} \rho_{sb} \partial x} \left(k_s A \frac{\partial T_s}{\partial x} \right) + \left(\frac{a_{sg} \cdot h_{sg}}{C_{ps} \cdot \rho_{sb}} \right) (T_g - T_s) + \left(\frac{a_{xs} \cdot h_{xs}}{C_{ps} \cdot \rho_{sb}} \right) (T_x - T_s) \\ &\quad + \left(\frac{a_{sg} \cdot K_g}{C_{ps} \cdot \rho_{sb}} \right) (p_k - p_{ks}) \cdot (\Delta H_k) \end{aligned} \quad (2-7)$$

This equation is subject to the conditions

$$\frac{\partial T_s}{\partial x} = 0 \text{ at } x = 0$$

$$\frac{\partial T_s}{\partial x} = 0 \text{ at } x = x_0 \quad (2-8)$$



Energy Equation for Coolant Stream

$$\frac{\partial T_c}{\partial t} = -u_c \frac{\partial T_c}{\partial x} + \left(\frac{a_{vc} \cdot h_{xc}}{c_{pc} \cdot \rho_c} \right) (T_x - T_c) \quad (2-9)$$

The boundary condition for this equation is

$$T_c = T_{268} \text{ at } x = x_{\text{coolant inlet}} \quad (2-10)$$

Energy Equation for Heat Exchanger Core Metal

$$(c_{px} \cdot \rho_x) \frac{\partial T_x}{\partial t} = \frac{\partial}{\partial x} \left(k_x \frac{\partial T_x}{\partial x} \right) + a_{vx} \cdot [h_{xs} (T_s - T_x) + h_{xg} (T_g - T_x) + h_{xc} (T_c - T_x)] \quad (2-11)$$

Boundary conditions for this equation are

$$\frac{\partial T_x}{\partial x} = 0 \text{ at } x = 0 \text{ and } x = x_o \quad (2-12)$$

Absorption Material Balance Equation for k-th Component in Gas Stream

By neglecting axial diffusion and assuming that quasi-steady-state conditions exist for the gas phase material balance, the following is obtained.

$$\frac{dp_k}{dx} = \frac{P \cdot M_g}{f \cdot \rho_g \cdot u_g} \cdot a_{sg} \cdot K_g \cdot (p_{ks} - p_k) \quad (2-13)$$

This has an inlet condition

$$p_k = p_{k,\text{inlet}} \text{ at } x = x_o \quad (2-14)$$

Pressure Equation for Desorption

During the desorption cycle, both the bed pressure and gas flow rate vary with time and the axial location in the bed, and a method of calculating instantaneous pressures at various bed locations is desired. Although a quasi-steady-state assumption could be made regarding pressure calculations, the simplified problem obtained would still be a boundary value problem that requires an iterative method of solution. An alternative approach would be to solve a transient equation describing pressure changes. The latter approach was taken in the present program, and the derivation of the pressure-equation employed in the program is given below.



A material balance for a unit volume of bed gives

$$Af \left(\frac{\partial C}{\partial t} \right) = - \frac{\partial}{\partial x} (f \cdot C \cdot A \cdot u_g) + A \cdot \dot{M}_{sg} \quad (2-15)$$

$$\text{where } \dot{M}_{sg} = a_{sg} \cdot K_g \cdot (p_{ks} - p \cdot x_k) \quad (2-16)$$

and u_g is related to pressure gradient by

$$u_g = - \frac{1}{F} \left(\frac{\partial P}{\partial x} \right) \quad (2-17)$$

Also, by differentiating the perfect gas law

$$C = \frac{P}{RT_g} \quad (2-18)$$

one obtains

$$\frac{\partial C}{\partial t} = \frac{1}{RT_g} \left(\frac{\partial P}{\partial t} \right) - \left(\frac{P}{RT_g^2} \frac{\partial T_g}{\partial t} \right) \quad (2-19)$$

By combining Equations (2-17), (2-18), and (2-19), and dropping the term $\frac{P}{RT_g^2} \left(\frac{\partial T_g}{\partial t} \right)$, Equation (2-15) can be converted to Equation (2-20) in a quasi-isothermal condition:

$$\frac{\partial P}{\partial t} = \frac{P}{F} \left(\frac{\partial^2 P}{\partial x^2} \right) + \frac{P}{f \cdot C \cdot A} \frac{\partial}{\partial x} \left(\frac{A \cdot f \cdot C}{F} \right) \left(\frac{\partial P}{\partial x} \right) + \frac{P}{C \cdot f} \dot{M}_{sg} \quad (2-20)$$

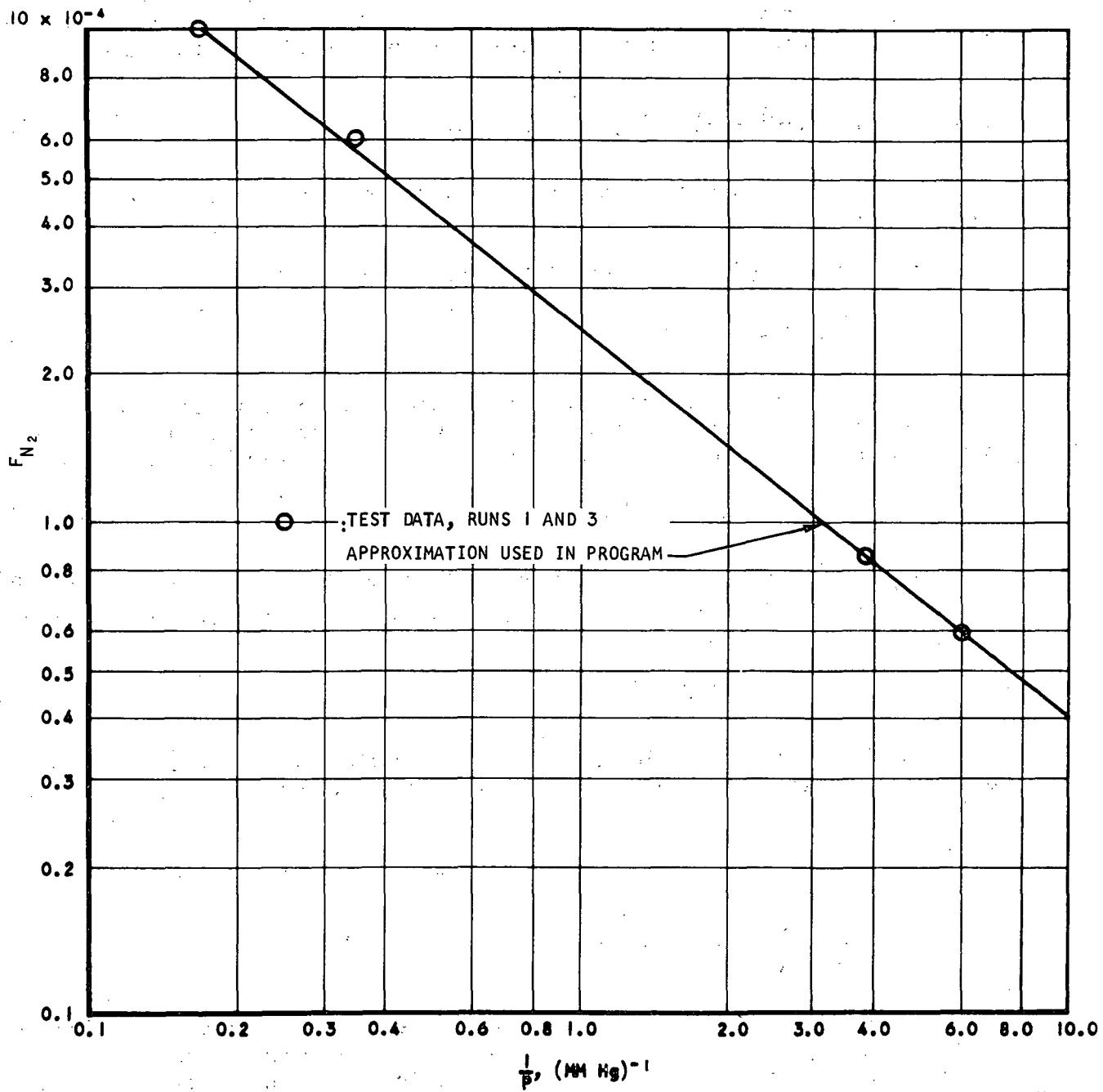
Equation (2-20) is used in the program for calculating pressure changes during the desorption half cycle.

The proportionality constant F in Equation (2-17) is a strong function of pressure, as the gas flow during desorption lies in the slip flow region. The pressure drop data for the flow of nitrogen gas through a 5/8-in.-ID molecular sieve bed were reduced by using the equation

$$\frac{F_{N_2} G.R.T_g}{M_g} = \frac{(P_1^2 - P_2^2)}{2(x_2 - x_1)} \quad (2-21)$$

to obtain F_{N_2} at various mean pressures. The result is plotted in Figure 2-1 and a best straight line fit of the data gives



Figure 2-1. Correlation of F_{N_2} vs $(\frac{1}{P})$ From Test Data72-8786
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$$F_{N_2} = 2.494 \times 10^{-4} \times P^{0.795} \quad (2-22)$$

Equation (2-22) is applicable only for nitrogen gas at 70°F, which has a viscosity of 0.0174 cp. In the desorption program, F is linearly corrected for the difference in viscosity as predicted by the Blake-Kozeny equation.

Thus $F = \left(\frac{\text{Avg Viscosity}}{0.0174} \right) \cdot 2.494 \cdot 10^{-4} \cdot P^{0.795}$ (2-23)

For the gas mixtures in the desiccant bed section, molal average viscosities were used in the program.

Equation (2-20) is subject to a boundary condition

$$\frac{\partial P}{\partial x} = 0 \text{ at } x = 0 \quad (2-24)$$

At the bed exit, the pressure can be specified as a function of time, or else the vacuum duct resistance to gas flow will play a role in fixing the pressure and flow rate. The boundary condition will then be

$$f \cdot \rho_g \cdot u_g \cdot A = W_D(P) \quad (2-25)$$

where $W_D(P)$ can be approximated by the following expression which corresponds to the straight line shown in Figure 2-2 for a 3-in. duct for the AAP vacuum duct.

$$W_D(P) = 11.2 P^{1.715} \quad (2-26)$$

The dotted lines in Figure 2-2 were the estimated flow rates for 18 in. long ducts. The resistance contributed by the gas valve were not included in these calculations.

Combination of Equations (2-17), (2-25), and (2-26) yields

$$\frac{\partial P}{F \partial x} = \left(\frac{11.2 P^{0.715}}{f \cdot \rho_g \cdot A} \right) P \quad (2-27)$$

In addition to the equations listed above, an equilibrium relationship between vapor pressure, temperature, and sorbate loading is needed for each sorbate-sorbent combination. The relationship can be in equation or tabular form.



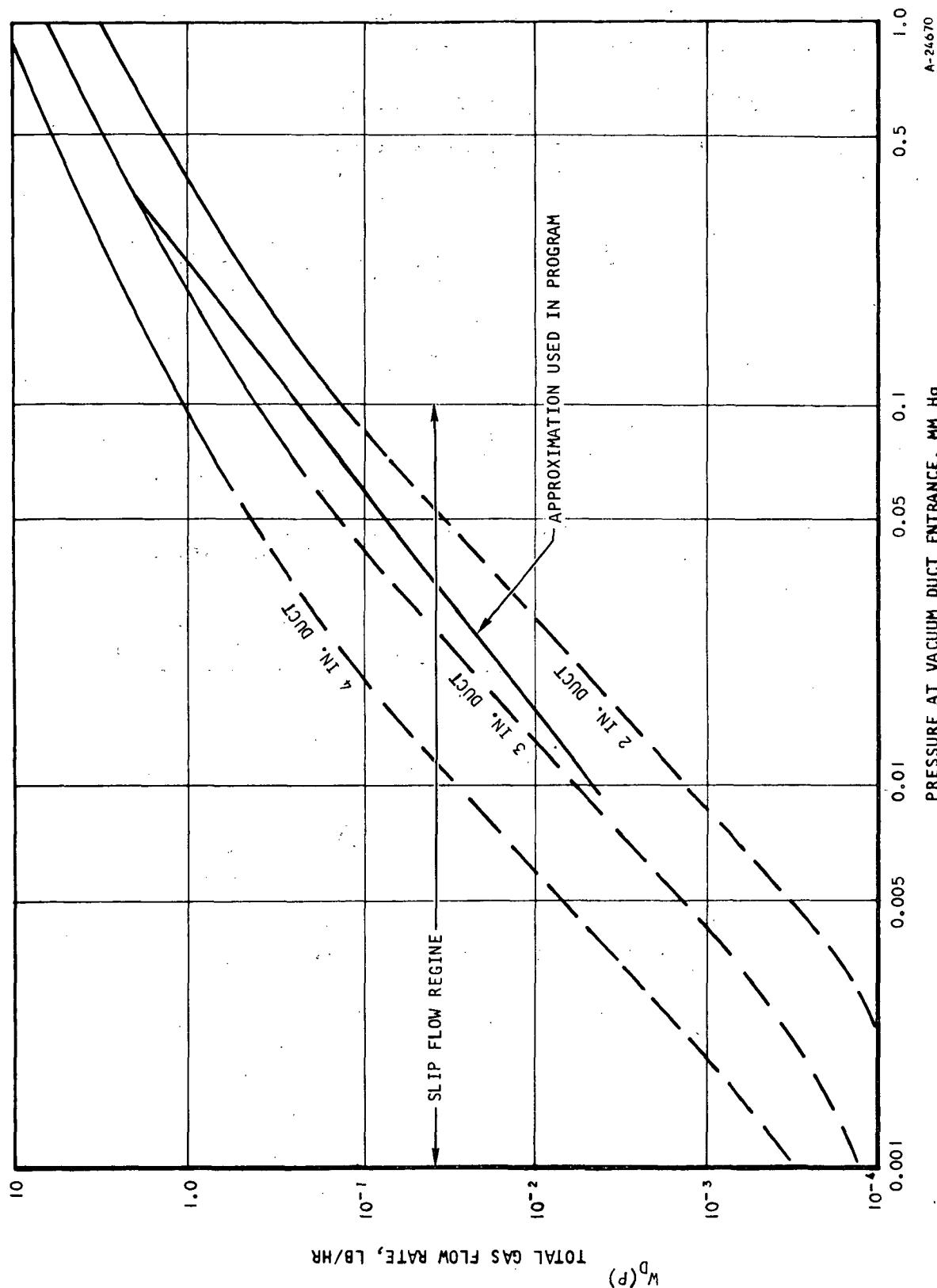


Figure 2-2. Vacuum Duct Capacities for Various Duct Sizes and Duct Inlet Pressures



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FINITE DIFFERENCE MODEL

The foregoing differential equations were solved in the program, using the following finite-difference approximations.

Diffusion Equation for Interior of Sorbent Pellet

For accuracy, the sorbent is divided into constant volume elements rather than into ones with constant (Δr). Equation (2-1) can then be approximated by

$$\begin{aligned} (\Delta V) \rho_s \cdot \left[\frac{w_{k,M,(t+\Delta t)} - w_{M,k,t}}{\Delta t} \right] &= \rho_s D_k \cdot \frac{(4\pi \cdot r_{M-1/2}^2)}{(r_M - r_{M-1})} \\ &\quad \cdot (w_{k,(M-1)(t+\Delta t)} - w_{k,M,(t+\Delta t)}) \\ &\quad - \frac{\rho_s \cdot D_k (4\pi r_{M+1/2}^2)}{(r_{M+1} - r_M)} \cdot (w_{k,M,(t+\Delta t)} - w_{k,(M+1)(t+\Delta t)}) \end{aligned} \quad (2-28)$$

Half nodes are used at the center and the surface of spherical pellets, and Equation (2-28), with boundary conditions (2-2) and (2-3) super imposed becomes respectively

$$\frac{(\Delta V)}{2} \cdot \rho_s \frac{w_{k,1,(t+\Delta t)} - w_{k,1,(t+\Delta t)}}{\Delta t} = - \frac{\rho_s D_k (4\pi r_{1-1/2}^2)}{(r_2 - 0)} \quad (2-29)$$

and

$$\frac{(\Delta V)}{2} \cdot \rho_s \frac{w_{k,s,(t+\Delta t)} - w_{k,s,t}}{\Delta t} = - \frac{\rho_s D_k (4\pi \cdot r_{M_s-1/2}^2)}{r_s - r_{M_s-1}} \quad (2-30)$$

$$\begin{aligned} &\left[w_{k,(M_s-1),(t+\Delta t)} - w_{k,M_s,(t+\Delta t)} \right] \\ &- A_s \cdot M_k \cdot K_g \cdot (P_{ks} - P \cdot X_k)_{(t+\Delta t)} \end{aligned}$$



Energy Equation for Gas Stream

Equation (2-4) is approximated by

$$\frac{T_g(N+1) - T_g(N)}{(\Delta x)} = \frac{1}{f \cdot \rho_g \cdot C_{pg} \cdot u_g} \left[a_{sg} \cdot h_{sg} \cdot (T_s(N+1) - T_g(N+1)) \right. \\ \left. - T_g(N+1) \right] + a_{xg} \cdot h_{xg} (T_x(N+1) - T_g(N+1)) \quad (2-31)$$

for $u_g > 0$

For the case $u_g < 0$, which is the case during adsorption, the index (N+1) will be replaced by (N-1).

Energy Equation for Sorbent

The following finite difference representation for Equation (2-7) is used in the program.

$$\frac{T_s(t+\Delta t), N - T_s(t-\Delta t), N}{2 \cdot (\Delta t)} = \frac{1}{C_{ps} \cdot \rho_{sb} \cdot (\Delta x)^2 A_N} \cdot \left[k_s(N+1/2) \right. \\ \cdot A_{(N+1/2)} \cdot \left(T_s(t+\Delta t), (N+1) - T_s(t+\Delta t), N \right) - k_s(N-1/2) \cdot A_{(N-1/2)} \\ \cdot \left(T_s(t+\Delta t), N - T_s(t+\Delta t), (N-1) \right) + \left(\frac{a_{sg} \cdot h_{sg}}{C_{ps} \cdot \rho_{sb}} \right)_N \cdot T_{g,t,N} \\ - \frac{T_s(t+\Delta t), N + T_s(t-\Delta t), N}{2} \left] + \left(\frac{a_{xs} - h_{xs}}{C_{ps} \cdot \rho_{sb}} \right)_N \left[T_{x,t,N} \right. \right. \\ \left. - \frac{T_s(t+\Delta t), N + T_s(t-\Delta t), N}{2} \right] + \left(\frac{a_{sg} \cdot K_g}{C_{ps} \cdot \rho_{sb}} \right)_N \\ \cdot \left[p_{k_s}(t+\Delta t), N - p_{k_s}(t-\Delta t), N \right] \cdot (\Delta H_k)$$



Energy Equation for Coolant Stream

The program uses the finite-difference analog to Equation (2-9)

$$\frac{T_{c(t+\Delta t),N} - T_{c(t-\Delta t),N}}{2(\Delta t)} = -u_c \frac{T_{c(t+\Delta t),N} - T_{c(t+\Delta t),(N-1)}}{(\Delta x)} \quad (2-33)$$

$$+ \left(\frac{a_{vc} \cdot h_{xc}}{C_{pc} \cdot \rho_c} \right)_N \cdot \left[T_{x,t,N} - \frac{T_{c(t+\Delta t),N} + T_{c(t-\Delta t),N}}{2} \right]$$

Energy Equation for Heat-Exchanger Core Metal

$$(C_{px} \cdot \rho_x) \frac{T_{x(t+\Delta t),N} - T_{x(t-\Delta t),N}}{2 \cdot (\Delta t)} = \frac{1}{(\Delta x)^2} \cdot \left[k_x(N+1/2) \cdot \left(T_{x(t+\Delta t),N} \right. \right.$$

$$\left. \left. - T_{x(t+\Delta t),(N-1)} \right) - k_x(N-1/2) \cdot \left(T_{x(t+\Delta t),N} \right. \right.$$

$$\left. \left. - T_{x(t+\Delta t),(N-1)} \right) \right] + a_{vx} \cdot h_{xs}$$

$$+ \left\{ T_{s,t,x} - \frac{T_{x(t+\Delta t),N} + T_{x(t-\Delta t),N}}{2} \right\} + h_{xg} \cdot \left\{ T_{g,t,N} \right.$$

$$- \left. \frac{T_{x(t+\Delta t),N} + T_{x(t-\Delta t),N}}{2} \right\} + h_{xc} \cdot \left\{ T_{c,t,N} \right.$$

$$- \left. \frac{T_{x(t+\Delta t),N} + T_{x(t-\Delta t),N}}{2} \right\}$$

Adsorption Material Balance for K-th Component in Gas Stream

Equation (2-13) is approximated by

$$\frac{P_{k(N-1)} - P_{k(N)}}{(\Delta x)} = \left(\frac{P \cdot M_g}{f \cdot \rho_g \cdot u_g} \right) \cdot a_{sg} \cdot k_g \cdot (P_{ks(N-1)} - P_{k(N-1)}) \quad (2-35)$$

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Pressure Equations for Desorption

Equation (2-20) is represented by

$$\frac{P_{(t+\Delta t), N} - P_{t, N}}{(\Delta t)} = \frac{P_{t, N}}{F_{t, N} \cdot (\Delta x)^2} \left[P_{(t+\Delta t), (N-1)} - 2P_{(t+\Delta t), N} + P_{(t+\Delta t), (N+1)} \right] + \left(\frac{P}{f \cdot c \cdot A} \right)_{t, N} \cdot \frac{1}{2(\Delta x)^2} \left[\left(\frac{A \cdot f \cdot c}{F} \right)_{t, N} - \left(\frac{A \cdot f \cdot c}{F} \right)_{t, (N-1)} \right] \cdot \left[P_{(t+\Delta t), (N+1)} - P_{(t+\Delta t), (N-1)} \right] + \left(\frac{P}{c \cdot f} \right)_{t, N} \cdot a_{sg} \cdot K_g \cdot \left[P_{ks(t+\Delta t), N} - P_{(t+\Delta t), N} \cdot x_{k, t, N} \right] \quad (2-36)$$

The boundary condition expressed by Equation (2-27) can be put in the form

$$-\frac{P_{(NDX_1+1)} - P_{NDX_1}}{F \cdot (\Delta x)} = \left(\frac{11.2 P^{0.715}}{f \cdot \rho_g \cdot A} \right)_{NDX_1} P_{NDX_1} \quad (2-37)$$

METHOD OF SOLUTION

Most of the finite difference schemes described above are of the implicit form and require a special method of solution, which is described below.

The system of finite difference equations describing bed property changes for all nodes can be written in the form (Reference 3)

$$C_2 Y_{1,(t+\Delta t)} + C_3 Y_{2,(t+\Delta t)} = D_1 \quad (2-38)$$

$$C_1 Y_{(N-1),(t+\Delta t)} + C_2 Y_{N,(t+\Delta t)} + C_3 Y_{(N+1),(t+\Delta t)} = D_N \quad (2-39)$$

$$C_1 Y_{(NDX_1-1),(t+\Delta t)} + C_2 Y_{NDX_1,(t+\Delta t)} + C_3 Y_{(NDX_1+1),(t+\Delta t)} = D_{NDX_1} \quad (2-40)$$

The matrix of this linear system is tridiagonal and the following formulae which were first presented by Thomas,² are used for its solution:

$$B_1 = \frac{C_3}{C_2} \quad (2-41)$$

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$$B_N = \frac{C_{3N}}{\left(C_{2N} - C_{1N} B_{N-1} \right)} \quad (N = 2, 3, \dots, NDXI) \quad (2-42)$$

$$Q_1 = \frac{D}{C_{21}} \quad (2-43)$$

$$Q_N = \frac{\left(D_N - C_{1N} Q_{N-1} \right)}{\left(B_N - C_{1N} B_{N-1} \right)}, \quad (N = 2, 3, \dots, NDXI) \quad (2-44)$$

$$Y_{NDXI} = Q_{NDXI} \quad (2-45)$$

$$Y_N = Q_N - B_N Y_{N+1}, \quad [N = (NDXI-1), (NDXI-2), \dots, 1] \quad (2-46)$$

It should be noted that the index N appearing in the above equations can be replaced by index M for solving the interior diffusion Equation (2-28) with its boundary conditions.

Equation (2-35) for the adsorption period and Equation (2-36) for the desorption period are coupled with Equations (2-30) and (2-32) and a special method is needed, which is described below for the desorption period first because this is the more involved of the two cases.

Equilibrium surface vapor pressure at the end of a time step is approximated by

$$\begin{aligned} p_{k,s,(t+\Delta t)} &= p_{k,s,t} + (w_{k,s,(t+\Delta t)} - w_{k,s,t}) \left(\frac{\partial p_k^*}{\partial w_k} \right)_{T_s} \\ &\quad + (T_{s,(t+\Delta t)} - T_{s,t}) \left(\frac{\partial p_k^*}{\partial T_s} \right)_{w_{k,s}} \end{aligned} \quad (2-47)$$

The new surface loading can be expressed as a function of the gas phase pressure:

$$w_{k,s,(t+\Delta t)} = Q_s + D_2 \cdot P_{(t+\Delta t)} \quad (2-48)$$

where Q_s is the Q as expressed by Equation (2-44) for the pellet interior diffusion, with the term containing $P_{(t+\Delta t)}$ excluded from it.



Sorbent temperature change in one time step during the desorption period is written as:

$$T_{s,(t+\Delta t)} - T_{s,t} = D_s + C_{s1} \cdot P_{(t+\Delta t)} - C_{s2} \cdot P_{k,s(t+\Delta t)} \quad (2-49)$$

Substituting Equations (2-48) and (2-49) into Equation (2-47), the following is obtained

$$P_{k,s,(t+\Delta t)} = P_1 + P_2 \left[Q_s - W_{k,s,t} \right] + \left[P_2 \cdot D_2 + P_3 \right] \cdot P_{(t+\Delta t)} \quad (2-50)$$

where $P_1 = \left[P_{k,s,t} + D_s \left(\frac{\partial p_k^*}{\partial T_s} \right)_{W_k} \right] / \left[1 + C_{s2} \cdot \left(\frac{\partial p_k^*}{\partial T_s} \right)_{W_k} \right]$ (2-51)

$$P_2 = \left(\frac{\partial p_k^*}{\partial W_k} \right)_{T_s} \left[1 + C_{s2} \left(\frac{\partial p_k^*}{\partial T_s} \right)_{W_k} \right] \quad (2-52)$$

$$P_3 = C_{31} \cdot \left(\frac{\partial p_k^*}{\partial T_s} \right)_{W_k} \left[1 + C_{s2} \left(\frac{\partial p_k^*}{\partial T_s} \right)_{W_k} \right] \quad (2-53)$$

Now, Equation (2-36) can be rewritten as follows, where N designates the N-th axial node counted from the furthest end from the vacuum duct connection:

$$\begin{aligned} \frac{P_{N,(t+\Delta t)} - P_{N,(t)}}{(\Delta t)} &= P_{C1} \cdot \frac{P_{(N-1),(t+\Delta t)} - 2 \cdot P_{N,(t+\Delta t)} + P_{(N+1),(t+\Delta t)}}{(\Delta x)^2} \\ &+ P_{C2} \cdot \frac{P_{(N+1),(t+\Delta t)} - P_{(N-1),(t+\Delta t)}}{2 \cdot (\Delta x)} \\ &+ P_{C3} \cdot \left[P_{ks} - X_k \cdot P_{N,(t+\Delta t)} \right] \end{aligned} \quad (2-54)$$

The last term of this equation becomes, by the substitution of Equation (2-50):

$$P_{C3} \cdot \left[P_{ks} - X_k \cdot P_{N,(t+\Delta t)} \right] = C_{P1_N} + C_{P2_N} \cdot P_{N,(t+\Delta t)} \quad (2-55)$$



$$\text{where } C_{P1,N} = P_{C3,N} \cdot \left[P_{1N} + P_{2N} \cdot \{ Q_{sN} - w_{ks}(t) \} \right] \quad (2-56)$$

$$C_{P2,N} = P_{C3,N} \cdot \left[\{ P_{2N} \cdot D_{2N} + P_{3,N} \} - X_k \right] \quad (2-57)$$

Combining Equations (2-54) and (2-55) and rearranging, the following is obtained.

$$C_{1P,N} \cdot P_{(N-1), (t+\Delta t)} + C_{2P,N} \cdot P_{N, (t+\Delta t)} + C_{3P,N} \quad (2-58)$$

$$\cdots P_{(N+1), (t+\Delta t)} = D_{1P,N}$$

$$\text{where } C_{1P,N} = -\frac{P_{C1,N}}{(\Delta x)^2} + \frac{P_{C2,N}}{2 \cdot (\Delta x)} \quad (2-59)$$

$$C_{2P,N} = \frac{1}{(\Delta t)} + \frac{2 \cdot P_{C1,N}}{(\Delta x)^2} - C_{P2,N} \quad (2-60)$$

$$C_{3P,N} = \frac{P_{C1,N}}{(\Delta x)^2} - \frac{P_{C2,N}}{2(\Delta x)} \quad (2-61)$$

$$D_{1P,N} = \frac{P_{N,t}}{(\Delta t)} + C_{P1,N} \quad (2-62)$$

Equation (2-58) has P as the only unknown, and can be solved by the method using Equations (2-41) through (2-46). Once P 's are found, new loadings and temperatures can be obtained using these pressures.

For the adsorption period, by setting $X_k = 1$, and replacing P by p_k , Equation (2-36) by Equation (2-35), the following equations are obtained:

$$w_{ks,(t+\Delta t)} = Q_s + D_2 \cdot p_{k,(t+\Delta t)} \quad (2-64)$$

$$T_{s,(t+\Delta t)} - T_{s,t} = D_s + C_{s1} \cdot p_{k,(t+\Delta t)} - C_{s2} \cdot p_{k,s,(t+\Delta t)} \quad (2-65)$$

$$p_{k,s,(t+\Delta t)} = P_1 + P_2 [Q_s - w_{k,s,t}] + [P_2 \cdot D_2 + P_3] \quad (2-66)$$

$$\cdots p_{k,(t+\Delta t)}$$



$$P_{k,N,(t+\Delta t)} = \left[\frac{P_{k,(N+1),(t+\Delta t)}}{(\Delta x)} + \frac{C_{P1,N}}{\frac{f \rho_g \cdot u_g}{P \cdot M_g}} \right] \left[\frac{1}{(\Delta x)} \right] \quad (2-67)$$

$$- \left[\frac{C_{P2,N}}{\left(\frac{f \cdot \rho_g \cdot u_g}{P \cdot M_g} \right)} \right]$$

where $C_{P1,N} = a_{sg} \cdot K_g \cdot [P_1 + P_2 \cdot (Q_s - W_{k,s})]$ (2-68)

$$C_{P2,N} = a_{sg} \cdot K_g \cdot (P_2 \cdot D_2 + P_3 - 1) \quad (2-69)$$

Equation (2-67) is used to find P_k 's from the process gas inlet end all the way to the outlet end. W_k 's are found next, followed by temperatures.

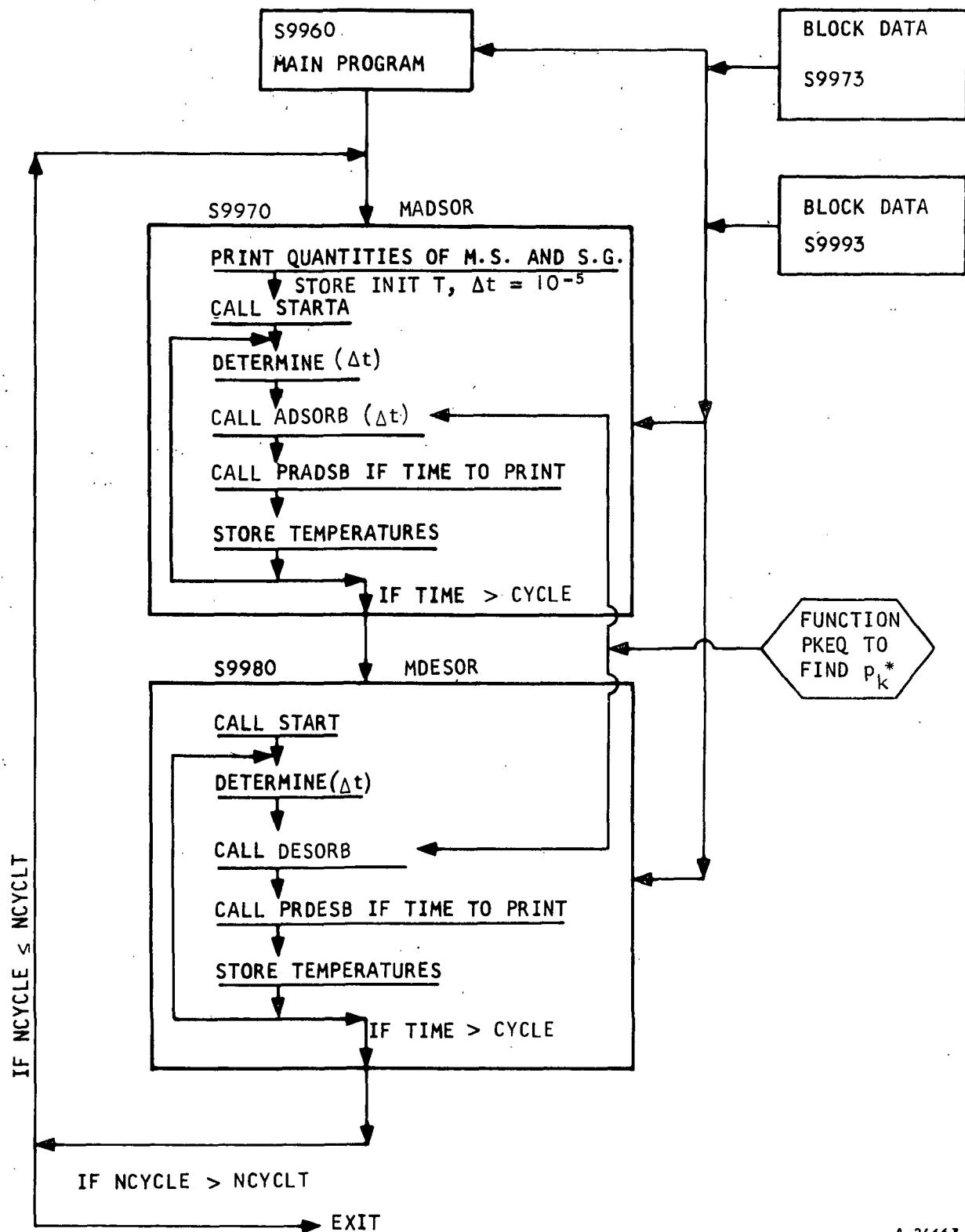
GENERAL FLOW CHART

A general flow diagram of S9960 is given in Figure 2-3.

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Figure 2-3. Structure of Program S9960

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SECTION 3

USAGE

PROGRAM INPUT

Data input required by the program is executed by block data subprograms S9973 and S9993. Subprogram S9973 inputs all data required to execute the adsorption analysis; subprogram S9993 inputs all data required to execute the desorption analysis. Both block data subprograms must be compiled at execution time if cyclic system performance is desired. If only adsorption or desorption performance is required, then only the respective block data subprogram need be compiled at execution time. The following lists the variables which are inputted via the block data subprograms.

Variables Common to Both S9973 and S9993

<u>FORTRAN Symbol</u>	<u>Maximum Dimension</u>	<u>Definition</u>
<u>Bed Configuration</u>		
ABED	(41)	Sorbent bed cross-section area normal to flow of process gas, sq ft
AGX	(41)	Identical to ASX
ASX	(41)	Heat exchanger primary area per unit volume of sorbent bed, sq ft/(cu ft)
DX		Axial node dimension, ft
NDR4		Integer denoting total number of radial sorbent pellet nodes (interior nodes)
NDXM		Integer denoting total number of molecular sieve nodes
NDXMAC		Integer denoting number of active molecular sieve nodes, i.e., (NDXM - NDXMAC) represents the number of molecular sieve nodes which have been inactivated by water poisoning
NDXI		Integer denoting total number of axial nodes



<u>FORTRAN Symbol</u>	<u>Maximum Dimension</u>	<u>Definition</u>
<u>Sorbent Properties</u>		
ASG	(41)	Sorbent specific surface area, sq ft/(cu ft of bed)
CPS	(41)	Sorbent specific heat, Btu/(lb) ($^{\circ}$ F)
RHOS	(2)	Sorbent particle density, lb/(cu ft) RHOS (1) = molecular sieve particle density, RHOS (2) = desiccant particle density
RHOSB	(41)	Sorbent bulk density, lb/(cu ft)
SK	(41)	Effective sorbent thermal conductivity, Btu/(hr) (sq ft) ($^{\circ}$ F/ft)
<u>Coolant Properties</u>		
AVC	(41)	Primary heat exchanger plate area per unit volume of coolant held up in HX, sq ft/(cu ft)
CPC	(41)	Coolant specific heat, Btu/(lb) ($^{\circ}$ F)
NOG		Node to which coolant is added
RHOC	(41)	Coolant density, lb/(cu ft)
T268		Coolant inlet temperature, $^{\circ}$ F
UC	(41)	Coolant velocity, ft/hr
<u>Heat Transfer Coefficients</u>		
HSG	(41)	Heat transfer coefficient, sorbent to gas, Btu/(hr) (sq ft)($^{\circ}$ F)
HXC	(41)	Heat transfer coefficient, heat exchanger to coolant Btu/(sq ft) (hr)($^{\circ}$ F)
HXG	(41)	Heat transfer coefficient, heat exchanger to process gas, Btu/(sq ft) ($^{\circ}$ F) (hr)
HXS	(41)	Heat transfer coefficient, heat exchanger to sorbent, Btu/(sq ft)(hr)($^{\circ}$ F)



<u>FORTRAN Symbol</u>	<u>Maximum Dimension</u>	<u>Definition</u>
<u>Initial Conditions</u>		
TC	(41)	Initial coolant temperature, $^{\circ}$ F
TG	(41)	Initial gas temperature, $^{\circ}$ F
TS	(41)	Initial sorbent temperature, $^{\circ}$ F
TX	(41)	Initial heat exchanger temperature, $^{\circ}$ F
W	(21,41)	Initial sorbent loading, lb/lb (double precision)
<u>Mass Transfer Properties</u>		
DIF	(41)	Internal diffusivity, sq ft/hr
GK	(41)	External surface mass transfer coefficient, lb-mole/(hr)(sq ft)(mm Hg)
<u>Process Gas Stream Properties</u>		
CPG	(41)	Specific heat of the process gas, Btu/(lb)($^{\circ}$ F)
DH	(41)	Differential heat of adsorption, Btu/(lb adsorbed)
WM	(2)	Adsorbate molecular weight WM(1) = 44 (CO_2) WM(2) = 18 (H_2O)
<u>HX Core Properties</u>		
AVX	(41)	Primary heat exchanger plate area per unit volume of heat exchanger core metal, sq ft/(cu ft)
CPX	(41)	Heat exchanger specific heat, Btu/ $^{\circ}$ F(lb)
RHOX	(41)	Heat exchanger metal density, lb/(cu ft)
TKX	(41)	Heat exchanger metal thermal conductivity, TKX (K) denotes that between node K-1 and node K, Btu/(hr)(sq ft)($^{\circ}$ F/ft)



<u>FORTRAN Symbol</u>	<u>Maximum Dimension</u>	<u>Definition</u>
<u>Miscellaneous Control Parameters</u>		
CYCLE		Cycle time per one adsorption or one desorption, period, hr
DTMAX		Maximum allowable time step size, usually 0.01 hr for isothermal analysis and 0.005 hr for nonisothermal analysis
NCYCLT		Total number of complete adsorption-desorption cycle calculations desired
NDTC ϕ N		If NDTC ϕ N = 1, Δt will be selected such that $\Delta T = TI$, $\Delta W = WI$ for time step; if NDTC ϕ N = 2, Δt 's as set in program will be used
NPRINT		Integer control variable which determines the frequency of printout occurrence; e.g., if NPRINT = 2, printout occurs after every two time steps, if NPRINT = 5, printout occurs after every five time steps, etc.
NTEMP		Integer control variable; if NTEMP = 0, isothermal analysis; the energy equations are ignored, and the bed temperature is set equal to T268. If NTEMP \neq 0, nonisothermal analysis
TI		Maximum temperature change allowable per time increment in selecting Δt , $^{\circ}$ F
WI		Maximum loading change allowable per time increment in selecting Δt , lb/lb

NOTE: Variables W, TG, TS, TC, TX, NPRINT, DTMAX, NTEMP, CYCLE, NCYCLT, WI, TI, NDXMAC and NDTC ϕ N need to appear only once either in S9973 or S9993.



Input Variables Required by S9973 Only

<u>FORTRAN Symbol</u>	<u>Definition</u>
GMR	Process gas flow rate, lb/hr
GMW	Process gas molecular weight
PA	System total pressure, mm Hg
PC _{02C}	Initial CO ₂ partial pressure in cabin, mm Hg
PH _{2O1}	Inlet H ₂ O partial pressure, mm Hg
TGI	Inlet process gas temperature, °F
V _{LCAB}	Cabin volume for atmosphere, cu ft; use V _{LCAB} = 10 ²⁰ , for constant PC _{02C}
RC _{02C}	Rate of CO ₂ generation in cabin, lb CO ₂ per hr

Input Variables Required by S9993 Only

<u>FORTRAN Symbol</u>	<u>Definition</u>
NBCOUT	Integer control variable; if NBCOUT = 2, the outlet manifold pressure is specified as a function of time; NBCOUT = 1, the manifold pressure is computed from vacuum duct resistance
POUT (10) TIMET (10)	10 pairs of exit pressure vs time data to be used if NBCOUT = 2; POUT = vacuum end manifold pressures (mm Hg), TIMET = times (hr)
NPSET (3)	Denotes nodes to which vacuum is applied

Function PKEQ (ID, W,T), S9992

This function subprogram must be defined, which computes for ID = 1, the equilibrium CO₂ pressure over the molecular sieve sorbent at a loading of W lb CO₂/lb sieve and at T °F; and for ID = 2, computes H₂O vapor pressure over the desiccant sorbent at a loading of W lb H₂O/lb desiccant and T °F.



Equilibrium isotherms can be used in tabular forms and p_k^* obtained by an interpolation technique, or the data can be fit by a mathematical expression which is evaluated in this subprogram. The latter approach is recommended since experience has indicated that by using the former approach, the total run time of the present program is about twice the time required by using the latter approach.

Vacuum Duct Characteristics

The vacuum duct characteristics represented by Equation (2-26) was for a 3-in.-ID by 18 in. long duct, which may not be the case for the problem to be simulated. If this is the case the outlet boundary condition expressed by Equations (2-26) and (2-37) must be modified. The required changes are minor and will be shown in the example problem to be presented in Section 4.

OUTPUT DESCRIPTION

The first page of output gives bed volumes and weights of molecular sieves and desiccants.

From the second page on, bed properties are printed at the end of each adsorption and desorption period. From the NSTART-th cycle on, the bed properties are printed every NPRINT time steps.

In the adsorption period, the cycle number is printed on the first line. Time from the beginning of adsorption period is printed next in hours and minutes. The size of time increment last used follows the adsorption time. CO_2 and H_2O partial pressures in the process gas stream, gas, sorbent, coolant, and HX core temperatures are then given at each axial node, node 1 designating the bed outlet and the highest node representing the process gas inlet node. Sorbate loadings in (lb sorbate)/(lb sorbent) appear at all sorbent interior nodes and at all axial locations. The average loading at each axial location is also given. The average CO_2 loading in the active molecular sieve sorbent, the average H_2O loading in the desiccant sorbent, average rates of CO_2 and H_2O adsorption computed over the period from the beginning of the adsorption cycle up to the moment, time average water partial pressure at the bed outlet, and the average rate of H_2O influx into the CO_2 -sorbent section are printed.

Printouts during desorption periods are similar to those of adsorption periods except that, for all longitudinal locations total pressures instead of the partial pressures of CO_2 and H_2O are printed, and in addition, mole fractions of H_2O in the vapor phase and molal flow rates of CO_2 and H_2O for all axial nodes, are also written.



EXECUTION CHARACTERISTICS

Restrictions

The program is limited in the case where sorbents are regenerated by vacuum desorption, either with or without the application of heat in addition. Program modifications will be required if gas stripping is resorted for sorbent regenerations.

The program requires a total of 31,000 words storage with Univac 1108 computer.

Running Time

Running time depends on the total number of nodes employed in a simulation. Using a total of 18 nodes, the ratio of real time to Univac 1108 computer time is roughly 150 to 1.

Accuracy/Validity

The present program was tested on the regenerable CO₂ removal systems for AAP and Airlock applications. Comparisons between the predictions made by the program and the test data are reasonably good.



SECTION 4

SAMPLE PROBLEM SOLUTION

BED DESIGN

As an example of the program usage, the performance of the CO₂-removal system designed by AiResearch for the Airlock application will be simulated. The bed design is shown in Figure 4-1.

The predryer section is bulk packed with Linde Molecular Sieves type 13X of 1/16 in. size. The CO₂ adsorber is composed of an electrically heated plate-fin heat exchanger, with the gas passages filled up with Linde Molecular Sieves type 5A of 1/16 in. size. The electric heater is used only for bakeout, and during normal operation the heat exchanger, together with the heater, simply acts as a thermal capacitor only. The electric heater elements used are KAPTON and the plate-fin heat exchanger is aluminum. The outside shell of the canister is made of stainless steel.

DESCRIPTION ON GENERATION OF INPUT DATA

The input data for simulating the performance of the above CO₂ removal unit are described below. Since no coolant is used for temperature control in the present system, coolant nodes are used as ambient temperature nodes to simulate heat losses to the surroundings, and the thermal capacitance of the heater is lumped into sorbent nodes. Heat exchanger core metal nodes designate the shell temperatures.

Bed Configuration

AVX = 375.0 is obtained by dividing the shell area by shell volume

ASX = AGX = 6.18 is obtained by dividing shell area by bed volume

ASG = 700 for bulk packed 1/16 in. pellets,

= 560 for same pellets in heat exchanger section

Heat Transfer CoefficientsI. Sorbent to Gas

HSG = 20 during adsorption. This is obtained from the low Reynolds number calculations of Pfeffer (Reference 4). The Nusselt number with a flow rate of 10.0 lb/hr is about 8.2. With a gas phase thermal conductivity of 0.01475

$\frac{\text{Btu}}{\text{hr ft}^2 \text{F}}$ and an effective particle diameter of:

$$d = \frac{6 \times 45}{64 \times 700} = 0.00603 \text{ ft},$$

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MOLECULAR SIEVE CANISTER COMPUTER NODAL STRUCTURE

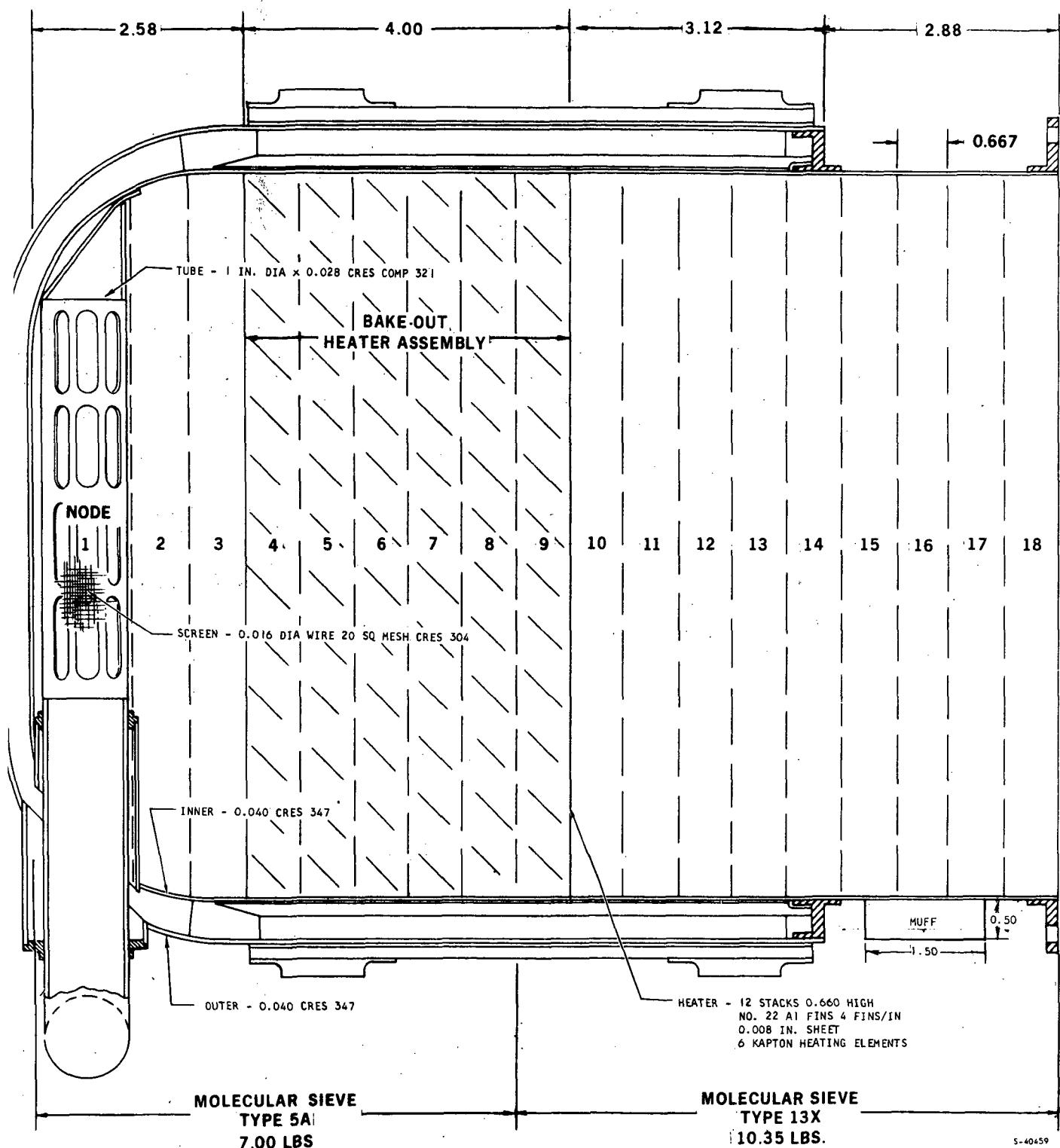


Figure 4-1. Molecular Sieve Canister for Airlock Application

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$$HSG = Nu \times k/d = 8.2 \times 0.01475/0.00603 = 20$$

During desorption, the thermal conductivity of the gas drops to 0.0022 Btu/hr ft $^{\circ}$ F, (Reference 5). Thus, HSG becomes

$$HSG = 8.2 \times 0.0022/0.00603 = 3.0$$

2. Sorbent to Shell

The term HXS accounts for all heat exchange between the sorbent and the canister wall. To make these calculations, the effective thermal conductivity of the sorbent must be known. (This is also necessary for the term SK.) Phillips (Reference 6) has obtained a correlation for bed thermal conductivity as a function of the gas conditions as well as the sorbent.

For the conditions here during adsorption:

$$SK = 0.10 \text{ Btu}/(\text{sq ft})(\text{hr})(^{\circ}\text{F}/\text{ft})$$

and for desorption,

$$SK = 0.08 \text{ Btu}/(\text{sq ft})(\text{hr})(^{\circ}\text{F}/\text{ft})$$

The conductivity in the heater section is then estimated by using volume weighted average of heater and sorbent conductivities. During adsorption,

$$SK = 11.6$$

and during desorption,

$$SK = 11.6$$

The heat transfer coefficients are found by assuming a conductance path. In the bulk pack sections the path is taken as one-half the distance from the canister wall to the center of the bed. This yields a coefficient during adsorption of,

$$HXS = k/\Delta X = 0.10/0.145 = 0.685$$

during desorption,

$$HXS = 0.08/0.145 = 0.55$$

In the heat exchanger core the same conductance path was used. However, the mixed Al-MS conductivity is used. During adsorption the coefficient becomes

$$HXS = 11.6/0.146 = 79.5$$

during desorption, the coefficient is

$$HXS = 11.6/0.146 = 79.5$$



3. Gas to Shell

The gas to shell heat exchange accounts for a very small portion of the total energy transfer. The coefficient is calculated throughout the canister as the conductivity divided by the average heat path.

$$HXG = 0.01475/0.146 = 0.101$$

during desorption

$$HXG = 0.0022/0.146 = 0.0151$$

Diffusion Coefficients for CO₂ in 5A and H₂O in 13X

DIF = 4.0×10^{-4} throughout. No internal mass transfer resistance results from the use of this size diffusion coefficient.

Mass-Transfer Coefficients

The following mass transfer coefficients are determined from test data obtained at AiResearch.

1. Adsorption

$$GK_{CO_2 - 5A} = 0.9 \times 10^{-4}$$

$$GK_{H_2O - 13X} = 5.0 \times 10^{-3}$$

2. Desorption

$$GK_{CO_2 - 5A} = 5.0 \times 10^{-4}$$

$$GK_{H_2O - 13X} = 1.0 \times 10^{-3}$$

Properties of Sorbents

1. Sorbent Density

$$RH\phi S = 64 \text{ lb/cu ft}$$

2. Bulk Density

$$RH\phi SB = 45 \text{ lb/cu ft in bulk pack}$$

$$RH\phi SB = 36 \text{ lb/cu ft in heater core}$$



Heat of Adsorption

The following heat of adsorption data are calculated from equilibrium isotherm data as described in (Reference 7).

$$\Delta H = 400 \text{ for } CO_2 \text{ on } 5A \text{ (Btu/lb)}$$

$$\Delta H = 1400 \text{ for } H_2O \text{ on } 13X \text{ (Btu/lb)}$$

Equilibrium Data

Equilibrium data for $H_2O - 13X$ and $CO_2 - 5A$ are fitted by equations and are used in FUNCTION PKEQ.

Vacuum Duct and Gas Valve Characteristics

The gas discharge capacity of the vacuum duct with gas valve for the Airlock molecular sieve system was found to be approximated by the following expression:

$$W_D(P) = \left[\ln\left(\frac{P}{0.888}\right) + 1.76 \right] / 1.96 \quad (4-1)$$

This equation is used in subroutine DESORB for the present simulation.

SUMMARY AND LISTING OF INPUT DATASummary of Input Data

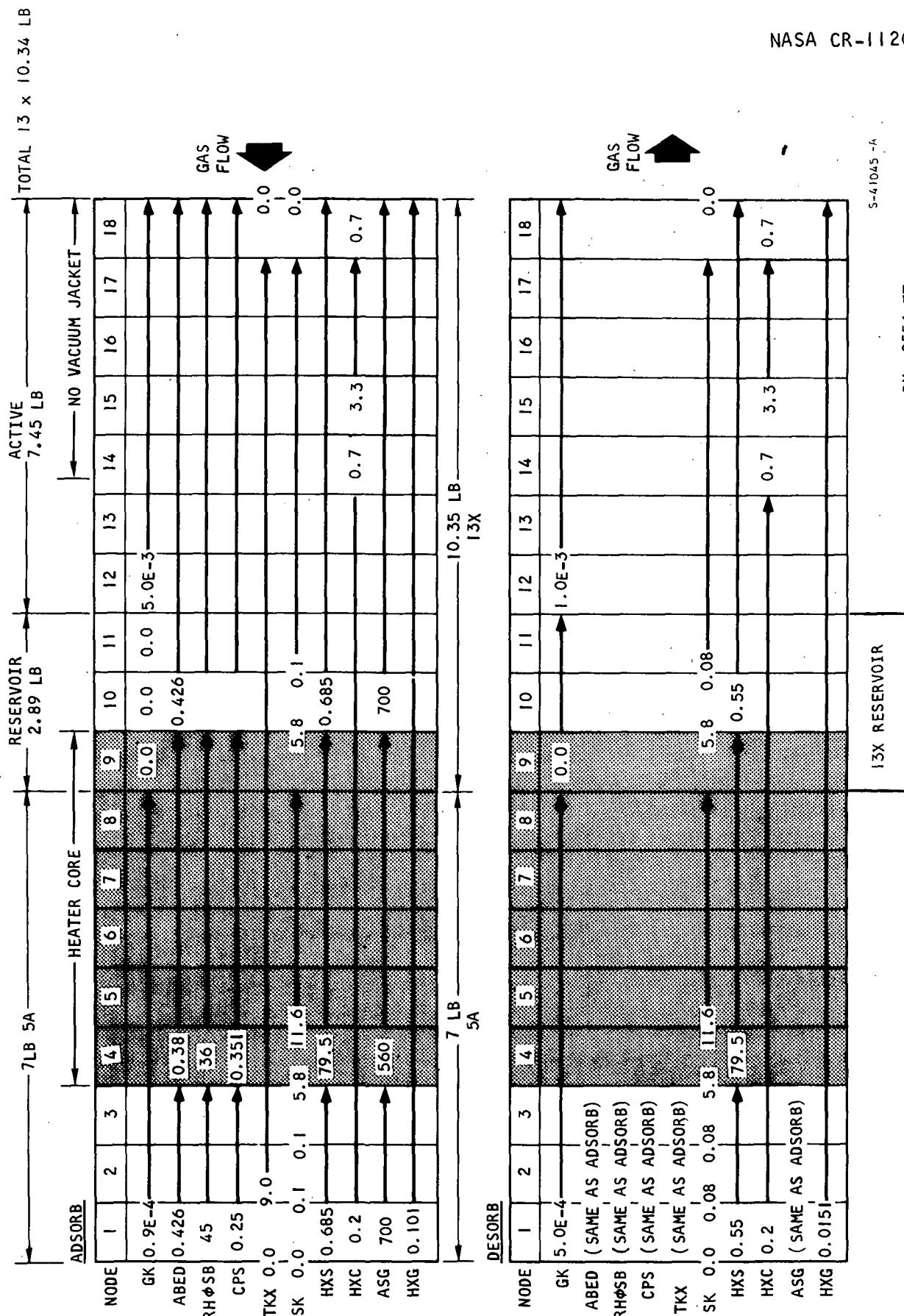
A summary of the input data for the example problem is presented in Figure 4-2.

Listings of the input and output data are given in the following pages.

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INPUT DATA FOR EXAMPLE PROBLEM

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000001      C   BLOCK DATA
000002      C   INPUT DATA TO ADSORB
000003      COMMON /BLOK2/ ABED(41), A(41), AVC(41), CPG(41), RHOG(41),
000004      IHXG(41), HXS(41), HYC(41), DIF(41), OF(41), VS(41), DS(2), DS(1), R
000005      2S1(2,41), RHOS(2), DG(41), UC(41), NDXM, PS(41), RHOSB(41), DS(41),
000006      3CS1(41), CS2(41), C1(21,41), C2(21,41), D1(21,41), D2(41), PC1(41),
000007      PC2(41), PC3(41), ASC(41), ASX(41), AGX(41), C2P(41), C3P(41), D1P(41),
000008      5, FR(2,41), RS(2), NDXI, NDRA, DX, DT, GK(41), DH(41), SK(41), P1(41),
000009      6, P3(41), WS(41), CR(2,21), CR(2,21), CR(2,21), C3(21,41), B(21,41),
000010      7G(21,41), CP1(41), CP2(41), X(41), VD1F(41), TIME
000011      8, AXC(41), RHOC(41), CPC(41), T268, AVX(41), TKX(1), CPX(41), RHOX(41)
000012      9, NOG, PK(2,41), PCO21, PW201, GMR GMW TGL, PA, PT(41), CPS(41), HSG(41)
000013      COMMON /BLOK3/ W(21,41), TC(41), TS(41), TC(41), X(41), CYCLE
000014      DOUBLE PRECISION W
000015      COMMON /BLOK6/ NCYCLT
000016      COMMON/BLOK10/ NPRINT,DTMAX,NDTCN
000017      COMMON /BLOK12/ NTEMP
000018      COMMON /BLOK13/ WI, TI
000019      COMMON /BLOK14/ NDXMAC, PC02C, VOLCAB, RC02C
000020      COMMON /BLOK17/ NSTART
000021      DIMENSION AXS(41), AXG(41), AGS(41), HSX(41), HGX(41), ACX(41),
1HGX(41)
000022      EQUIVALENCE (AXS,AXG), (AGX,AXG), (AGS,AGS), (HSX,HSX), (HGX,HGX)
000023      1, HGS) (LXC,ACX), (HXC,HCX)
000024      C   BED CONFIGURATION
000025      C
000026      C
000027      DATA ABED/3*426.6*38.9*426.23*0/, /
000028      DATA ND1, NDXM, NDXMAC, NDR4, DX / 18., 11., -8., -2., 0.0556/, /
000029      DATA AGX / 41*6.18/
000030      DATA AGS / 41*6.18/
000031      C   SORBENT PROPERTIES
000032      C   SORBENT PROPERTIES
000033      C
000034      DATA AGG/3*700., 6*560., 9*700., 23*0, 0/
000035      DATA CPS/3*25, 6*351, 9*25, 23*0, 0/
000036      DATA RHOS / 64., -64., /, /
000037      DATA RHOSB/3*45., 6*36., 9*5., 23*0, 0/
000038      DATA T268 / 70., /, /
000039      DATA SK/0.0, 2*1.5, 8.5*11.6, 5.8*8.8*1.23*0, 0/
000040      C   COOLANT PROPERTIES
000041      C
000042      DATA AVC / 41*100., /, /
000043      DATA CPC/41*1.E20/, /
000044      DATA NOG / 1., /, /
000045      DATA T268 / 70., /, /
000046      DATA UC41*0, 0/
000047      C   HEAT TRANSFER COEFFICIENTS
000048      C
000049      DATA HSG / 41*20., /, /
000050      DATA HXC/13*0.2, 7.3*3.3, 7.23*0, 0/
000051      DATA HXG/18*0.101, 23*0, 0/
000052      DATA HXS/3*, 685, 6*79.5, 9*, 685, 23*0, 0/
000053      C   INITIAL CONDITIONS
000054      DATA TC/14*70., 3*65., 24*70, 0/
000055      DATA TG/8.55., 3*75., 3*80., 75., 60., 40., 23., 23*50., /
000056      DATA TS/8*55., 3*75., 3*80., 75., 60., 40., 23., 23*50., /
000057      DATA TX/41*70., /

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000059      DATA * /16A*, 03100, 63*1.0-3, 21*, 1200, 21*, 13700, 21*, 1500, 21*, 1600,
000060      C MASS TRANSFER PROPERTIES
000061      C
000062      DATA DIF/41*4.E-4/
000063      DATA GK /8*0.9E-4, 3*0.0, 7*5.E-3, 23*0.0 /
000064      C PROCESS GAS STREAM PROPERTIES
000065      C
000066      DATA CPG / -41*0.23 /
000067      DATA OH / 11*400., 7*1400., 23*0.0 /
000068      DATA WM / 44.0, 18.0 /
000069      C HXCORE PROPERTIES
000070      C
000071      DATA AVX /41*375./
000072      DATA CPX / 41*0.11/
000073      DATA RHDX/ /41*490./
000074      DATA TKX / .0. 17*9.0 23*0.0 /
000075      C MISCELLANEOUS CONTROL PARAMETERS
000076      C
000077      DATA CYCLE/ 0.25/
000078      DATA NTEMP/ 1/
000079      DATA NCYCLT, NSTART/10.10/
000080      DATA NPRINT/10/
000081      DATA WI,TI/ 0.005, -1.5 /
000082      DATA DTMAX/ 0.008 /
000083      DATA NDTCN/ 1 /
000084      C ADSORB PARAMETERS
000085      C
000086      DATA PCO2C, PH2O1, TGI /7.0, 10, 52, /
000087      DATA VOLCAB, RCO2C / 320.0, 0.281, /
000088      DATA GMRCMW/10., 28.04/
000089      DATA PA/258. /
000090      END

```

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```

000001      BLOCK DATA
000002      C INPUT DATA TO DESORB
000003      COMMON /BLOK1/ 4BED(41), A(41), CPG(41), RHOG(41),
000004      1HXC(41), HXS(41)HXC(41), C(41), VS(2), DVS1(2), R
000005      2S1(2,41), RHOS(2,41), UC(41), NDXM, PS(41), DS(41),
000006      3CS1(41), CS2(41), C1(21,41), C2(21,41), D1(21,41), D2(41), PC1(41),
000007      41), PC3(41), ASG(41), ASX(41), AGX(41), C1P(41), C2P(41), C3P(41), D1P(41)
000008      5, FR(2,41), RS(2) NDXI, NDR4, DX, DT, GK(41), SK(41), P1(41), P2(41),
000009      6, P3(41), WS(41), CR1(2,21), CR2(2,21), CR3(2,21), C3(21,41), B(21,41),
000010      70(21,41), CP1(41), CP2(41), Y(41), VO1DF(41), TIME
000011      8, AXC(41), RHQC(1), CPC(41), T26A, AVX(1), JKX(41), CPX(41), RHXM(41)
000012      9, NOG, PK(2,41), PC021, PH201, GMR, GMW, TGI, PA, PT(41), CPS(41), MSG(41)
000013      DOUBLE PRECISION C1,C2,D1D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,
000014      1, C1, C2, D1D2, PC1, PC2, PC3, P1, P2, P3, C3, Q, B,
000015      COMMON /BLOK3/ W(21,41), TG(41), TS(41), TC(41), TX(41), CYCLE
000016      DOUBLE PRECISION W,
000017      COMMON /BLOK4/ POUT(10), NMBCOUT, NPSET(3)
000018      COMMON /BLOK5/ NCYCLT
000019      COMMON /BLOK10/ NPRINT, DTMAX, NDTCON
000020      COMMON /BLOK12/ NTEMP
000021      COMMON /BLOK13/ WI, TI
000022      COMMON /BLOK16/ NDXMLAC, PC02C, VOLCAB, RC02C
000023      COMMON /BLOK17/ NSTART
000024      DIMENSION AXS(41), AXL(41), AOS(41), HSX(41), HGX(41), ACX(41),
000025      1HXC(41)
000026      EQUIVALENCE (ASX,AXS), (AGX,AXG), (ASG,AGS), (HSX,HSX), (HGX,HGX), (MSG
000027      1, MSG), (AXC,ACX), (HXC,HCX)
000028      C BED CONFIGURATION
000029      C
000030      C
000031      C
000032      DATA ABED/30.426,60.38,9.426,-230.0/
000033      DATA NDXM, NDXMLAC, NDRA, DX / 10, 11, 6, 2, 0.0556/
000034      DATA AGX / 41*6,18/
000035      DATA ASX / 41*6,18/
000036      C SORBENT PROPERTIES
000037      C
000038      DATA ASG/3*700.,6*560.,9*700.,23*0.0/
000039      DATA CPS/3*25.6*351.,9*25,23*0.0/
000040      DATA RHOS/64., 64. /
000041      DATA RHOSB/3*45.,6*36.,9*45.,23*0.0/
000042      DATA SK/0.0,28.08,5.8,5*13.6,5.8,08,23*0.0/
000043      C COOLANT PROPERTIES
000044      DATA AVC / 41*100. /
000045      DATA CPC/41*1.E20/
000046      DATA NOG / 1 /
000047      DATA T268 /70. /
000048      DATA UC/41*0.0/
000049      C HEAT TRANSFER COEFFICIENTS
000050      C
000051      DATA MSG /41*3.0 /
000052      DATA HXC/13*0.2,7.3*3.3,7.23*0.0/
000053      DATA HXG/18*0.051,23*0.0,0.0/
000054      DATA HXS/30.55,6*79.5,9.55,23*0.0/
000055      C MASS TRANSFER PROPERTIES
000056      C
000057      DATA DIF/41*4.E-4/
000058      DATA GK/8*5.E-4,3*0.0,7*1.E-3,23*0.0/

```



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```
000059          C PROCESS GAS STREAM PROPERTIES
000060
000061          DATA CPG / 41*0.23 /
000062          DATA DH / 11*400., 7*1400., 23*0.0 /
000063          DATA WM / 44.0, 18.0 /
000064          C HXCORE PROPERTIES
000065          DATA AVX / 41*375. /
000066          DATA CPX / 41*0.11 /
000067          DATA QHOX/ 41*490. /
000068          DATA TKX / 0. 17*9.0, 23*0.0 /
000069
000070          C DESORB PARAMETERS
000071          DATA NBCOUT/ 1/
000072          DATA NPSET / 0.0, 18/
000073          END
000074
```

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• ELT S9992,1,690501, 43774

```

FUNCTION PKEQ(W,L,W,T)
PKEQ=EQUILIBRIUM PRESSURE IN MM HG
ID=2,420 ON 13X
10=1,C02 ON MOLECULAR SIEVE 5A
W=LOADING IN LB ADSORBATE PER LB ADSORBENT
T=TEMP IN DEG F
DATA B1/ 070523D784 /
DATA B2/ .0422820123 /
DATA B3/ .0092705272 /
DATA B4/ .0001520143 /
DATA B5/ .0002765672/
DATA B6/ .0000430638/
C
IF (W .LE. 0. ) W= 1.E-5
GO TO (41.51),1D
41 CONTINUE
Y ALOG (W)
YBIG=D.667*Y*2.22*0.0025*T
H=ABS(YBIG)
IF (H .GE. 1.0) GO TO 231
IF (H-.000011 15,15,16
15 XBIG=1.7725*H/2.0
GO TO 18
16 CONTINUE
IELH=.LE.-0.84) GO TO 1
IF (H .LE. 0.88) GO TO 2
IF (H .LE. 0.934) GO TO 3
IF (H .LE. 0.984) GO TO 4
IF (H .LE. 0.997) GO TO 5
XD=2.2*200. *(H-0.998)
GO TO 6
231 H=1.0
GO TO 17
1 X0=H
GO TO 10.6
2 X0=1.0
GO TO 10.6
3 X0=1.2
GO TO 6
8 X0=1.3+8. *(H-.934)
GO TO 6
5 X0=1.7+30. *(H-.984)
6 HPRXD=(2./1.77245)*EXP(1.* (X0)*#2)
C=16.
HNEW=1.+X0*(B1*X0*(R2*X0*(B3*X0*(B4*X0*(B5*X0*(B6))))))
HNEW=1.+-NEW*#C
DELH=H-HNEW
TERM=DELH/HPRXO
XBIG=X0+TERM+X0*TERM*#2+(1.*X0*#2+1.)*TERM*#3)/3.+{(7.*X0*#12.
*X0*#3)*TERM*#4/6.
GO TO 18
17 XBIG=4.0
18 XBIG=SIGN(XBIG)*YBIG
12 X(BIG=0.493+0.00953*T)/0.38
PKEQ=EXP(X)
RETURN
51 CONTINUE
PKEQ=EXP((7.2*w-1.31E4/(T+460.))+15.2)

```

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RETURN!
END

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000060

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OUTPUT DATA FOR EXAMPLE PROBLEM



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TOTAL VOLUME OF M.S. BED = .2452 CU FT
TOTAL WT OF M.S. BED = 9,693 LB
TOTAL VOLUME OF S.G. BED = .1658 CU FT
TOTAL WT OF S.G. BED = 7,461 LB
TOTAL WT OF ACTIVE M.S. BED = 7,001 LB

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ADSORPTION CYCLE 3
TIME = .25000 HR 15.000 MIN TIME INCREMENT = .00010 HR

AXIAL NODE	PCO ₂ , MM	PH2O, MM	GAS TEMP, F	SORBENT TEMP, F	COOLANT TEMP, F	HX CORE TEMP, F
1	2.9659	.0266	73.5514	73.5399	69.9999	72.4927
2	3.3260	.0266	75.2208	75.2119	69.9999	73.1577
3	3.7410	.0266	76.5122	76.5127	69.9999	74.3898
4	4.2411	.0266	76.4586	76.4590	69.9999	76.2045
5	4.7296	.0266	76.4202	76.4211	69.9999	76.3174
6	5.3091	.0266	76.3211	76.3228	69.9999	76.2339
7	5.9265	.0266	76.1422	76.1446	69.9999	76.0612
8	6.5029	.0266	75.8939	75.8965	69.9999	75.8128
9	6.8842	.0266	75.6331	75.6358	69.9999	75.4556
10	6.8842	.0266	75.3529	75.3643	69.9999	75.9867
11	6.8842	.0266	73.7137	73.7079	69.9999	73.0192
12	6.8842	.0266	73.5609	74.5223	69.9999	72.6148
13	6.8842	.0266	80.1246	79.9936	69.9999	72.8505
14	6.8842	.0266	99.0533	98.8847	69.9999	73.5828
15	6.8842	.0266	123.3266	123.5668	64.9999	73.9740
16	6.8842	.0266	118.0636	118.1930	64.9999	73.2868
17	6.8842	.0266	99.6914	99.8166	64.9999	72.5691
18	6.8842	.0266	76.9300	79.1171	69.9999	72.6501

LOADING AT INTERIOR OF SORBENT, LB/LB

SORB NODE	Avg	1	2	3	4	5	6	7	8	9	10	11
1	.0356	.0356	.0357									
2	.0369	.0369	.0370									
3	.0385	.0384	.0386									
4	.0408	.0407	.0409									
5	.0433	.0431	.0434									
6	.0466	.0464	.0467									
7	.0506	.0504	.0507									
8	.0531	.0530	.0532									
9	.0610	.0610	.0610									
10	.0010	.0010	.0010									
11	.0010	.0010	.0010									
12	.1198	.1198	.1198									
13	.1364	.1364	.1365									
14	.1307	.1505	.1508									
15	.1708	.1705	.1710									
16	.1948	.1946	.1949									
17	.2462	.2161	.2163									
18	.2388	.2387	.2388									

AVG CO₂ LOADING IN M.S. BED = .9426 LB/LBAVG H₂O LOADING IN S,G. BED = .1753 LB/LBTIME AVG CO₂ ADSORP RATE = .2769 LB/HRTIME AVG H₂O ADSORP RATE = .2482 LB/HR

TIME AVG EXIT PH₂O = .0261 gm

TIME AVG RATE OF H₂S POISONING BY H₂O = .6495-03 LF H₂O/HR

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DESORPTION CYCLE 3
TIME = .25000 HR

TIME INCREMENT = .00106 HR



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AXIAL NODE	TOTAL PRESS, MM	GAS TEMP, DEG F	SORBENT TEMP, DEG F	COOLANT TEMP, DEG F	HX CORE TEMP, DEG F
1	1.7976	67.4260	67.4260	69.9999	68.3718
2	1.7859	66.5355	66.5353	69.9999	67.8291
3	1.7621	64.9264	64.9259	69.9999	66.7709
4	1.7261	65.0595	65.0596	69.9999	65.2339
5	1.6854	65.1453	65.1454	69.9999	65.1883
6	1.6349	65.2648	65.2649	69.9999	65.2970
7	1.5744	65.4216	65.4218	69.9999	65.4533
8	1.5036	65.6162	65.6164	69.9999	65.6368
9	1.4224	65.8453	65.8456	69.9999	66.0016
10	1.3297	66.0852	66.0854	69.9999	67.6673
11	1.2186	72.1368	72.1426	69.9999	68.9369
12	1.1049	73.9355	73.9373	69.9999	69.5487
13	9872	76.4363	76.6392	69.9999	69.4571
14	8639	78.0037	78.0054	69.9999	68.4589
15	72324	70.9618	70.9530	64.9999	66.2668
16	5901	54.5498	54.5321	64.9999	63.9891
17	4336	34.8350	34.8117	64.9999	61.7366
18	2574	15.6726	15.6465	69.9999	59.7297

AXIAL NODE	MOLE FRAC	CO ₂ RATE, M/MHR	H ₂ O RATE, M/MHR
1	1.00000	.000526	.000000
2	1.00000	.001054	.000000
3	1.00000	.001795	.000000
4	1.00000	.002332	.000000
5	1.00000	.002874	.000000
6	1.00000	.003426	.000000
7	1.00000	.003978	.000000
8	1.00000	.004521	.000000
9	1.00000	.004521	.000000
10	1.00000	.004521	.000000
11	1.00000	.004521	.000000
12	.017900	.004521	.000083
13	.051202	.004521	.000243
14	.111674	.004521	.000362
15	.191927	.004521	.001062
16	.274719	.004521	.001702
17	.345515	.004521	.002390
18	.426412	.004521	.003398

LOADING AT INTERIOR OF SORBENT

SORB NODE	AVG	1	2	3	4	5	6	7	8	9	10	11
AXIAL NODE												
1	.0323	.0323	.0322	.0322	.0326	.0326						
2	.0327	.0328	.0328	.0328	.0327	.0327						
3	.0338	.0339	.0339	.0339	.0337	.0337						
4	.0333	.0334	.0334	.0334	.0332	.0332						
5	.0328	.0329	.0329	.0329	.0327	.0327						

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6	.0322	.0322
7	.0313	.0314
8	.0303	.0304
9	.0010	.0010
10	.0010	.0010
11	.0010	.0010
12	.1194	.1194
13	.1356	.1356
14	.1482	.1482
15	.1633	.1633
16	.1834	.1834
17	.2038	.2038
18	.2238	.2237

Avg CO₂ Loading in M.S. Bed = .0324 LB/LB Avg H₂O Loading in S.G. Bed = .1682 LB/LB

Time Avg CO₂ Desorp Rate = .2843 LB/HR Time Avg H₂O Desorp Rate = .2135 LB/HR

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SECTION 5
REFERENCE INFORMATION

SUBPROGRAM DOCUMENTATION

Main Program (S9950)

This main program calls MADSOR to perform one adsorption half-cycle calculation.

Main Program (S9951)

This main program calls MDESOR to carry out one desorption half-cycle calculation.

MADSOR (S9970)

This subroutine monitors the adsorption half-cycle calculations. It prints the total quantities of molecular sieve and silica gel pellets in the composite bed for input data check-out purposes. The routine, then, calls STARTA. The time increment size for the next time step is selected such that TI and WI specified in the input data are satisfied. Subroutine ADSORB is then called to advance one time step, new cabin P_{CO_2} is calculated and the results are printed if this should be done according to NPRINT, and NSTART.

The program flow chart is given in Figure 5-1.

STARTA (S9978)

Everything which stays constant throughout the entire adsorption half cycle is evaluated in this subroutine. A, RS, CR1, CR2, CR3 are evaluated in the subroutine.

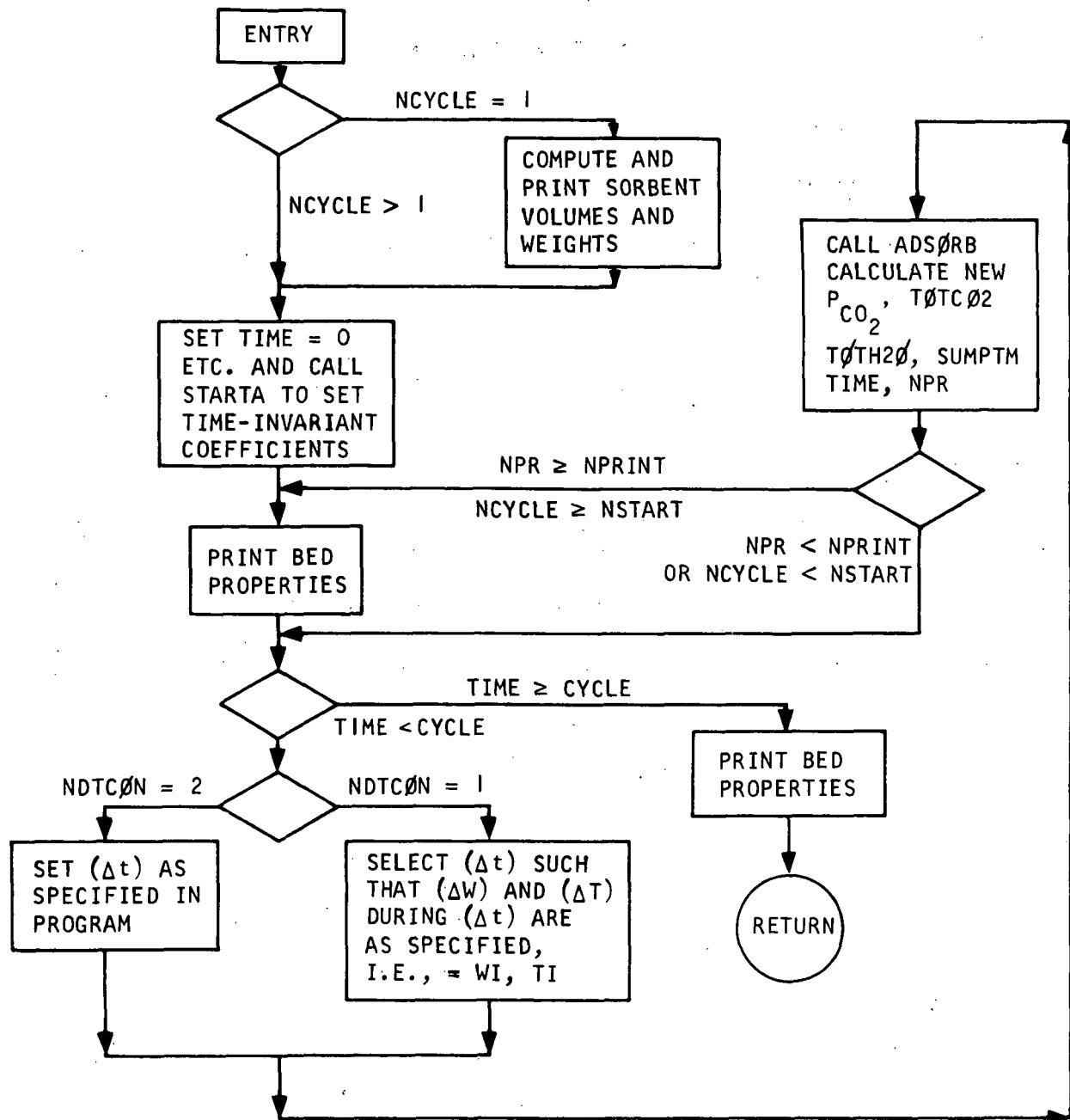
ADSORB (S9971)

This subprogram computes all the coefficients required in Equations (2-64) through (2-69), solve for p_k 's first, followed by bed loadings, and temperatures. A logic diagram of the subprogram is shown in Figure 5-2.

TSØRBA (S9977)

This routine solves Equation (2-32) for adsorption period sorbent temperatures, using the method shown in Equations (2-38) through (2-46).

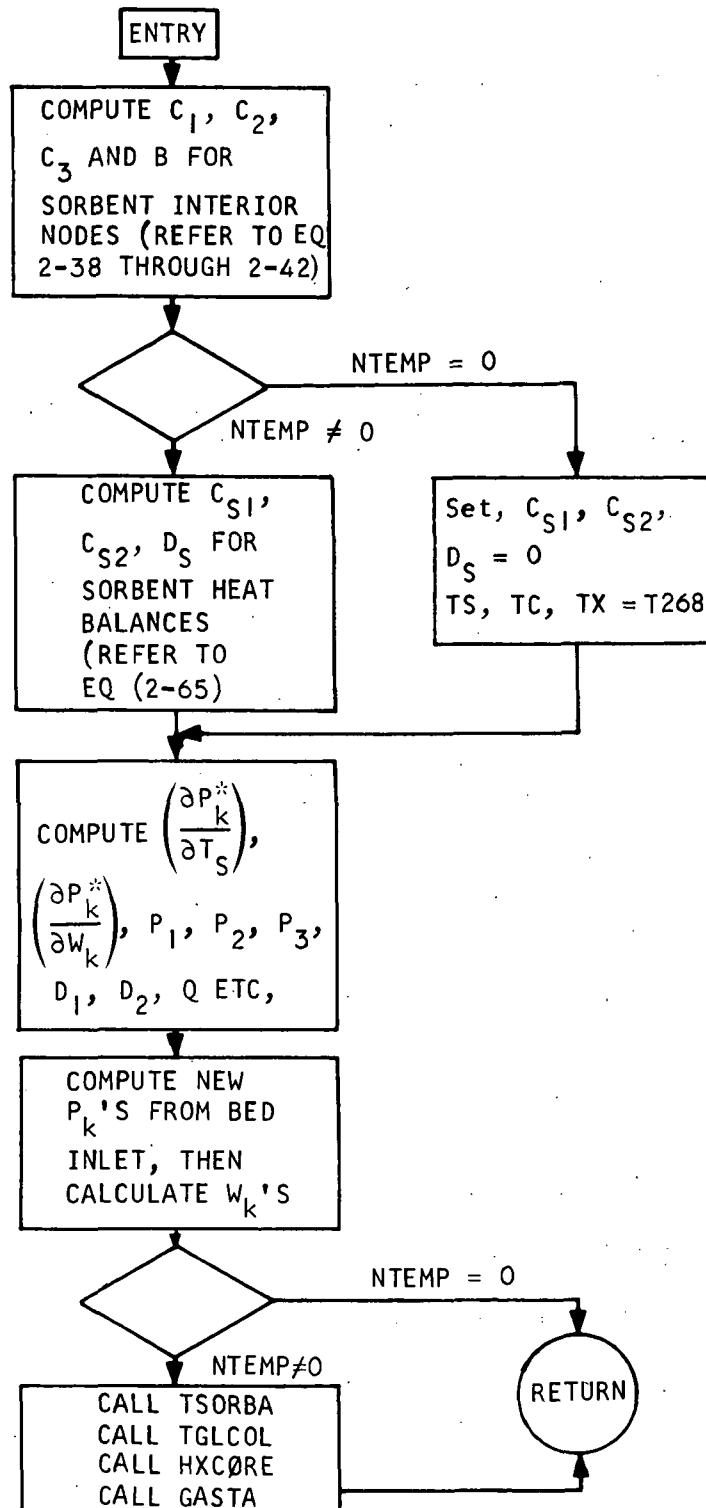




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Figure 5-1. Logic Flow Chart for MADSOR

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Figure 5-2. Logic Flow Chart for ADSORB

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TGLC0L (S9987)

Equation (2-33) is solved for coolant temperatures using the method described by Equations (2-38) through (2-46).

HXC0RE (S9991)

Equation (2-34) is solved for heat exchanger core temperatures using the method described in Equations (2-38) through (2-46).

GASTA (S9976)

Equation (2-31) is used to obtain gas temperatures for the adsorption period. Arguments of the subroutine are

CMR = process gas flow rate, lb/hr

CPG = specific heat of process gas stream, Btu/(lb)(°F)

ABED = cross-sectional area, (sq ft)

NDXI = total number of axial nodes

TGI = process gas inlet temperature, °F

ASG = sorbent surface area per unit bulk volume, (sq ft)/(cu ft)

HSG = heat transfer coefficient between gas and sorbent, Btu/(sq ft) (hr) (°F)

AXG = primary heat transfer area between heat exchanger and gas, (sq ft)/(cu ft)

HXG = heat transfer coefficient between heat exchanger and gas, Btu/(hr)(sq ft) (°F)

DX = axial increment size, ft

TG = gas temperature, °F

TS = sorbent temperature, °F

TX = heat exchanger temperature, °F

PRADSB (S9979)

This is the print routine for the adsorption program. A detailed description of output variables was given in Section 3.



MDESOR (S9980)

The routine controls desorption calculations much as MADSOR does the adsorption counterpart. It calls START, picks up a Δt , calls DESORB, PRDESB, and stores temperatures.

START (S9988)

Similar to STARTA for the adsorption, this subroutine generates all the coefficients which stay unchanged for the entire desorption half cycle.

PRDESB (S9989)

This is a print routine for the desorption program. For a detailed description of output variables, refer to Section 3.

DESORB (S9983)

Heat and material balance equations for the desorption period are solved by the method described in Section 2. The coefficients required in Equations (2-48) through (2-62) are computed, the desorption pressure Equation (2-58) is solved in double precision and these pressures are used to calculate new bed loadings and temperatures. A logic flow chart for this subprogram is given in Figure 5-3.

TSRB (S9997)

This routine solves for sorbent temperature in the desorption period, using the method described by Equations (2-38) through (2-46).

GAST (S9986)

The routine solves Equation (2-31) for the desorption period gas temperatures. Arguments of the subprogram are defined:

DX = axial increment size, ft

RHOG = density of vapor mixture, lb/(cu ft)

CPG = specific heat of vapor mixture, Btu/(lb)(°F)

U = linear velocity of vapor mixture, ft/hr

TS = sorbent temperature, °F

TX = heat exchanger temperature, °F

NDXI = total number of axial nodes

ASG = sorbent surface area per unit bulk volume, (sq ft)/(cu ft)

HSG = heat transfer coefficient between gas and sorbent, Btu/(hr)(sq ft)(°F)



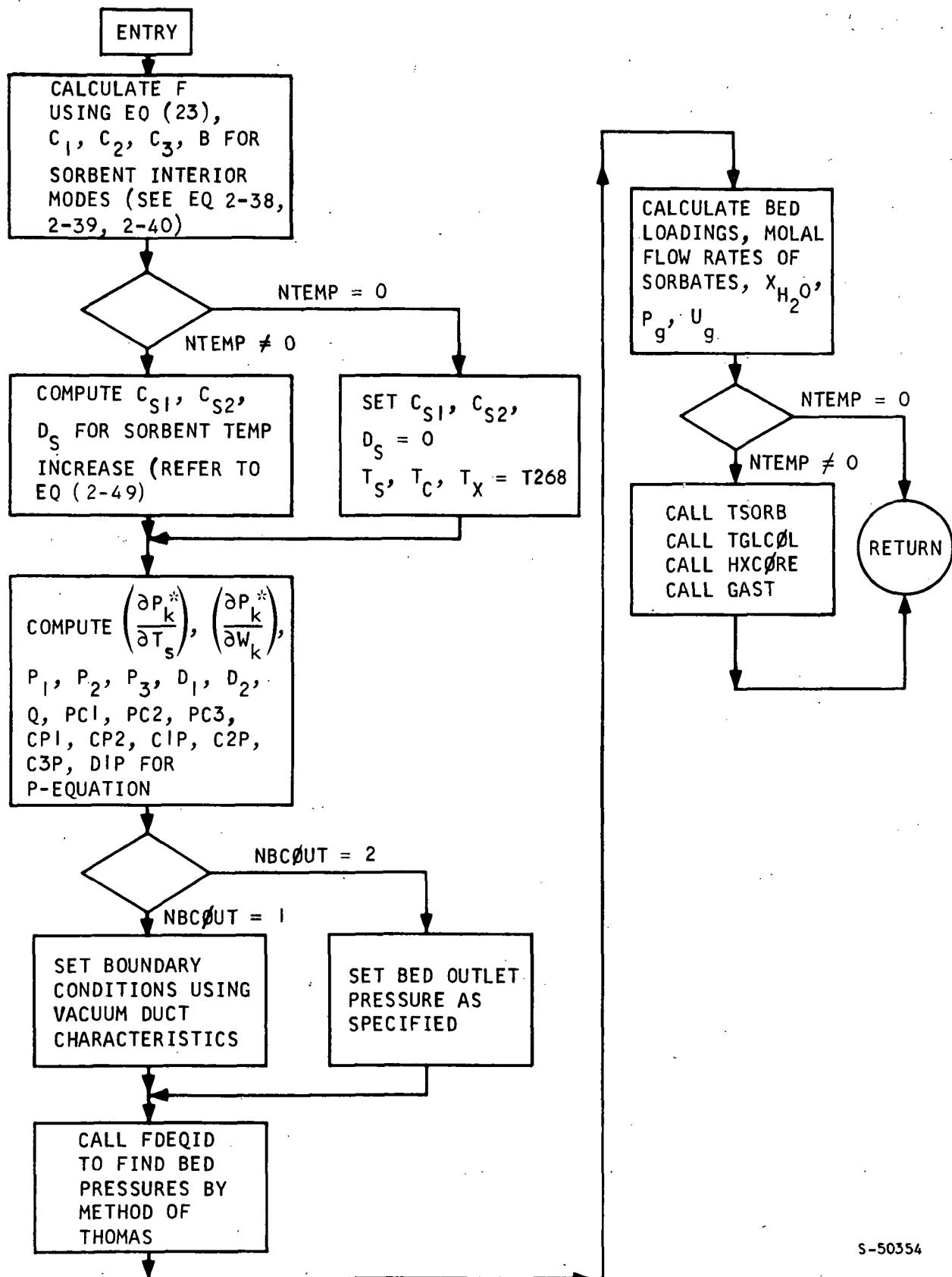


Figure 5-3. Logic Flow Chart for DESORB

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A_{HG} = primary heat transfer area between heat exchanger and gas,
 $(\text{sq ft})/(\text{cu ft})$

H_{HG} = heat transfer coefficient between heat exchanger and gas,
 $\text{Btu}/(\text{hr})(\text{sq ft})(^{\circ}\text{F})$

T_g = gas temperature, $^{\circ}\text{F}$

$V_f IDF$ = void fraction

PKEQ (S9992)

This function subprogram calculates the equilibrium CO_2 and H_2O vapor pressures over the molecular sieve and desiccant sorbents, respectively.

Arguments of the function are

ID = control index, $ID = 1$ indicates CO_2 over molecular sieve sorbent, $ID = 2$ indicates H_2O over desiccant sorbent.

w = loading, $\text{lb-sorbate}/(\text{lb-sorbent})$

T = sorbent temperature, $^{\circ}\text{F}$

IFN (S9981)

The function determines whether a given axial node belongs in the molecular sieve bed or desiccant bed.

FDEQIM (S9984)

The routine solves a system of finite difference equations by the method described by Equations (2-38) through (2-46).

FDEQID (S9985)

The subroutine is a double precision version of FDEQIM.

LAGIN2 (S9996)

This routine performs a Lagrangian polynomial interpolation. Arguments variables are:

ID = in case of trouble, this ID number will be printed for program checkout

X = independent variable

NP = number of tabulated pairs of data to be used



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ND = Number of points to be used in interpolation. For instance if
ND = 2, linear interpolation will be used

X ϕ = value of independent variable X

Y ϕ = value of dependent variable corresponding to X ϕ (this is the
answer obtained by LAGIN2)

Y = dependent variable



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SOURCE PROGRAM LISTING

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* ELT S9960,1,690501, 43778

```
000001      C MAIN PROGRAM FOR COMBINED ADSORPTION/DESORPTION PROGRAM -- DEVELOPED
000002      C BY K C HWANG, AIRESEARCH, LOS ANGELES
000003      C
000004      COMMON /BLOK3/ W(21,41),TG(41),TS(41),TC(41),TX(41),CYCLE
000005      DOUBLE PRECISION W
000006      COMMON /BLOK6/ NCYCLT
000007      COMMON /BLOK14/ NCYCLE
000008      NCYCLE=1
000009      11 CONTINUE
000010      WRITE (6,300)
000011      CALL MADSOR
000012      WRITE (6,400)
000013      CALL MDESCR
000014      NCYCLE=NCYCLE+1
000015      IF(NCYCLE .LE. NCYCLT) GO TO 11
000016      CALL EXIT
000017      300 FORMAT(2H1 START ADSORPTION CYCLE )
000018      400 FORMAT(2H1 START DESORPTION CYCLE )
000019      END
```



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U P D A T E

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• ELT S995D, 1-690501, 43776
CALL MADSOR
END
000001
000002

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* ELT 59951,1.690501, 43777
CALL MDESOR
END
000001
000002

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SUBROUTINE MADSSOR

```

000001      C
000002      COMMON /BLOK2/ ABED(41), A(41), AVG(41), CGC(41),
000003          1HXG(41), HXS(41), HXC(41), DIF(41), F(41), VS(2), DV51(2), R
000004          2S1(2,41), RHOSB(2), UG(41), WM(2), UC(41), NDXM(41), DS(41),
000005          3CS1(2,41), CS2(41), C1(21,41), C2(21,41), D1(21,41), PC1(4
000006          41), PC2(41), ASG(41), ASX(41), AGX(41), C1P(41), C2P(41),
000007          5, FR(2,41), RS(2), NDXI, NDRA, DX, DT, GK(41), DH(41), SK(41),
000008          P1(41), P2(41)
000009          6, P3(41), WS(41), CR1(2,21), CR2(2,21), C3(21,41), B(21,41),
000010          7G(21,41), CP1(41), CP2(42), X(42), VDF(41), TIME
000011          8, AXC(41), RHOC(41), CPC(41), T268, AVX(41), TKX(41), CPX(41), RHOX(41),
000012          9, NOG, PK(2,41), PC021, PH201, GMR, GMH, TGL, PA, PT(41), CPS(41), MSG(41)
000013          COMMON /BLOK3/ W(21,41), TG(41), TS(41), TC(41), TX(41), CYCLE
000014          DOUBLE PRECISION W
000015          COMMON /BLOK8/ DTO, TS1(41), TS2(41), TX2(41), TC1(41), TC2(41)
000016          COMMON /BLOK10/ NPRINT, DTMX, NDTCON
000017          COMMON /BLOK11/ TOTCO2, TOTH20, SUMPTM, WTACMS, WTSG
000018          COMMON /BLOK13/ W1, T1
000019          COMMON /BLOK14/ NCYCLE
000020          COMMON /BLOK16/ NDIMAC, PC02C, VOLCAB, RCC2C
000021          COMMON /BLOK17/ NSTART
000022
000023      IF(NCYCLE .GT. 1) GO TO 1
000024      N1=NDXM+1
000025      VMS=.0.
000026      WTMS=.0.
000027      VSGC=0.0.
000028      WSGA=0.0.
000029      JE(NDXM .EQ. 0) GO TO 11
000030      DO 10 N= 1, NDXM
000031      VMS=VMS+DX*ABED(N)*RHOSB(N)
000032      WTMS=WTMS+DX*ABED(N)*RHOSB(N)
000033      10 CONTINUE
000034      11 CONTINUE
000035      IF((NDXM-NDXM1).EQ. 0) GO TO 31
000036      DO 30 N= N1, NDXM1
000037      VSGEVSGDX*ABED(N)
000038      WSG=WTSG+DX*ABED(N)*RHOSB(N)
000039      30 CONTINUE
000040      31 CONTINUE
000041      WRITE(6,2001) VMS, WTMS, VSG, WTSG
000042      500 FORMAT(20H1 TOTAL VOLUME OF M.S. BED = G10.4,2X,5HCU FT//,
000043          12SH TOTAL WT OF M.S. BED = G10.4,2X,2HLB//,
000044          22SH TOTAL VOLUME OF S.G. BED = G10.4,2X,5HCU FT//,
000045          32SH TOTAL WT OF S.G. BED = G10.4,2X,2HLB)
000046      WTACMS=0.0
000047      IF(NDIMAC .EQ. 0) GO TO 12
000048      DO 70 N= 1, NDIMAC
000049      70 WTACMS=WTACMS +
000050      12 CONTINUE
000051      WRITE(6,501) WTACMS
000052      501 FORMAT( / 30H TOTAL WT OF ACTIVE M.S. BED = G10.4,3H LB )
000053      1 TIME = 0.0
000054      SUMPTM=0.
000055      DT=.1,E-5.
000056      DTO=.0.
000057      TOTCO2=0.0
000058      TOTH20=0.0

```



```

DC 20 N=1,NDX1
TS1(N)= TS(N)
TS2(N)= TS(N)
TX1(N)= TX(N)
TX2(N)= TX(N)
TC1(N)= TC(N)
TC2(N)= TC(N)
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000067
000068
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000117

20 CONTINUE
CALL STARTA
NPR=NPRINT - 1
GO TO 3
2 CALL PRADS
NPR = 0
4 CONTINUE
IF( TIME .GE. CYCLE) CALL PRADS
IF( TIME .GE. CYCLE) GO TO 9999
DT0=DT
DO 60 N=1,NDX1
ADT=0
/ABS((NDRA,N)-WS(N))+1.E-9)*DT
IF(ADT2,LT, ADT) ADT=ADT2
ADT2=1/(ABS( TS(N)-TS2(N))+1.E-9)*DT*2.0
IF(ADT2,LT, ADT) ADT=ADT2
ADT2=1/(ABS( TX(N)-TX2(N))+1.E-9)*DT*2.0
IF(ADT2,LT, ADT) ADT=ADT2
ADT2=1/(ABS( TC(N)-TC2(N))+1.E-9)*DT*2.0
IF(ADT2,LT, ADT) ADT=ADT2
60 CONTINUE
DT=ADT
GO TO 3
42 DT=DTMAX/10.0
IF(CTIME .GT. 0.06) DT=DTMAX
3 CONTINUE
IF((TIME+DT) .GT. CYCLE) DT = CYCLE-TIME
DO 21 N=1,NDX1
TS2(N)=TS1(N)
TS1(N)=TS(N)
TX2(N)=TX1(N)
TC2(N)=TC1(N)
TC1(N)=TC(N)
21 CONTINUE
PC021 = PC02C
CALL ADSORB(DT)
DPC02C = DT*(RC02C - GMRI)
1 (PC021-PK(1,1))*44./ (PA*GMW)+554.*5301/(44.*2VALCAB)
PC022C=PC02C+DPC02C
TOTC02=TOTC02-GMR*DT*(PC021-PK(1,1))*44./ (PA*GMW)
TDTH20=TOTH20-GMR*DI*(PK(2,0)-PK(2,1))*18./ (PA*GMW)
SUMPTM= SUMPTM+PK(2,1)*DT
TIME=TIME+DT
NPR = NPR+1
IF( (NPR.GE. NPRINT) .AND. (NCYCLE .GE. NSTART) ) GO TO 2
GO TO 4
9999 CONTINUE
RETURN
END

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      SUBROUTINE ADSORB(DELTA)
COMMON /BLOK2/ ABED(41), A(41), AVC(41), CGP(41), RHOG(41),
     1HXR(41), HXS(41), HXC(41), DIF(41), VS12, DV51(2), R
     2S1(2,41), RHOS(2), W1(2), UC(41), NDXM, PS(41), RHOSB(41), DS(41),
     3CS1(41), CS2(41), C1(21,41), C2(21,41), D1(21,41), D2(41), PC1(41),
     41) PC3(41), ASG(41), ASY(41), AGX(41), CIP(41), C2P(41), C3P(41), D1P(41)
     5, FR(2,41), RS(2), NDA1, NDR4, DT, GK(41), DH(41), P1(41), P2(41)
     6, PR(41), HS(41), CR1(2,21), CR2(2,21), CR3(2,21), C3(21,41), R(21,41),
     7Q(21,41), CP1(41), CP2(41), X(41), VOIDF(41), TIME
     8, AXC(41), RHOC(41), CPC(41), T268, AVX(41), TKX(41), CPX(41), RHOX(41),
     9, NOG, HK(2,41), PC021, PM201, GMR, GMW, GI, PA, PT(41), CPS(1), HSG(41)
COMMON /BLOK3/ W(21,41), TG(41), TS(41), TC(41), TX(41), CYCLE
      DOUBLE PRECISION W
COMMON /BLOK8/ DTO, TS1(41), TS2(41), TX1(41), TX2(41), TC1(41), TC2(41)
COMMON /BLOK12/ NTEMP
DIMENSION AS(2)
EQUIVALENCE (ASX, AXS), (AGX, AGS), (HXS, HSX), (HXR, HGX), (HSG
     1, HGS)
      DT = DELT
      AS(1)=3.1415926535897931160022
      AS(2)=3.1415926535897931160022
C
C
      DATA RGAS/594./
C
      NDR=NDR4+1
      DO 21 N=1,NDX1
      1=IFN(N,NDXM)
      DO 20 NR1, NDR4
      C1(NB,NJ)=CR2(J,NR)
      C2(NR,N)=CR1(I,NR)/DT+CR2(I,NR)*CR3(I,NR)
      20 C3(NR,N)=CR3(I,NR)
C
      B(1,N)=C3(1,N)/C2(1,N)
      DO 21 J=2,NDR
      21 B(J,N)=C3(J,N)/(C2(J,N)-C1(J,N)*B(J-1,N))
      NDX=NDX1-1
      TO TEMPORARILY STORE SURFACE LOADING
      DO 50 N=1,NDX1
      50 WS(N)=W(NDR4,N)
      IF (NTEMP.EQ.0) GO TO 111
C
      C      TO CALCULATE CS1,CS2,DS FOR SORBENT HEAT BALANCE EQUATION
      DO 12 N=1,NDX1
      1=IFN(N,NDXM)
      CS2(N)=DT/CP5(N)/RHOSB(N)*AGB(N)*GK(N)*WM(1)*DH(N)
      CS1(N) = CS2(N)
      IF (N.EQ.1) S1
      1=(ABED(N)+BED(N+1))*SK(N+1)*(TS(N+1)-TS(N))
      1=(ABED(N)*ABED(N+1))*SK(N+1)*(TS(N+1)-TS(N))
      2/(2.*ABED(N)*DX*DX)
      IF (N.EQ.1) GO TO 15
      S1=((ABED(N-1)+BED(N))*SK(N)*(TS(N-1)-TS(N))+
      1*(ABED(N)+BED(N+1))*SK(N+1)*(TS(N+1)-TS(N)))
      2/(2.*ABED(N)*DX*DX)
      15 DS(N)=DT/CP5(N)/RHOSB(N)*S1+ASC(N)*TS(N)-0.5*TS2(N)+1
      14SX(N)=HXS(N)*(TX(N)-0.5*TS2(N))+
```



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000059
000060      RATIO = (DT+DT0)/DT
000061      T1=(DT+DT0)/CPS(N)/RHOSB(N)
000062      T1=0.5*(ASG(N)*HSG(N)+ASX(N)*HXS(N))
000063      CS1(N)=RATIO*CS1(N)/(1.+T1)
000064      CS2(N)=RATIO*CS2(N)/(1.+T1)
000065      DS(N)=(DS(N)-T1)*TS2(N)/(1.+T1)
000066      112 CONTINUE
000067      GO TO 110
000068      111 DO 112 N= 1, NDX1
000069      CS1(N)=0,
000070      CS2(N)=0,
000071      DS(N)=0,
000072      TS(N)=T268
000073      TC(N)=T268
000074      TX(N)=T268
000075      TG(N)=T268
000076      112 CONTINUE
000077      110 CONTINUE
000078      C TO CALCULATE PARTIAL PRESSURE OF ADSORBATE IN GAS STREAM
000079      C
000080      DO 24 N=1,NDXA
000081      I=1FN(N,NDXM)
000082      C TO CALCULATE P1,P2,P3
000083      WSURF=W(NDR4,N)
000084      PSURF=PKEQ(1,WSURF,TS2(N))
000085      DPKOTS=DPKOTS/
000086      1(PKEQ(1,WSURF,(TS2(N)-0.001))-PSURF)/
000087      20.001
000088      DPKWK=(PKEQ(1,(WSURF+1.E-6),TS2(N))-PSURF)/1
000089      1.E-6
000090      G-1.+CS2(N)*DPKOTS
000091      P1(N)=(PSURF
000092      P2(N)=DPKWK/G
000093      P3(N)=CS1(N)/G*DPKOTS
000094      C
000095      C2(NDR4,N)=CR1(1,NDR4)/DT+CR2(1,NDR4)+WM(1)*GK(N)*P2(N)*AS(1)
000096      C3(NDR4,N)=0.0
000097      DO 23 NR=1,NDR4
000098      D1(NR,N)=CR1(1,NR)/DT+W(NR,N)
000099      D1(NDR4,N)=D1(NDR4,N)-AM(1)*GK(N)*(P1(N)-P2(N))*W(NDR4,N)*AS(1)
000100      D1(NDR4,N)=D1(NDR4,N)-AM(1)*GK(N)*(P1(N)-P2(N))*W(NDR4,N)*AS(1)
000101      D2(N)=AS(1)*WM(1)*GK(N)*(1.-P3(N))
000102      D2(N)=D2(N)*G2(NDR4,N)-C1(NDR4,N)*B(NCR4-1,N)
000103      Q1,N)=D1(1,N)/C2(1,N)
000104      DO 24 J=2,NDR4
000105      Q(J,N)=(D1(J,N)-C1(J,N)*Q(J-1,N))/(C2(J,N)-C1(J,N)*B(J-1,N))
000106      C
000107      DO 25 N=1,NDX1
000108      I=IFN(N,NDXM)
000109      CP1(N)=ASG(N)*GK(N)*(P1(N)+P2(N)*(Q(NDR4,N)-W(NDR4,N)))
000110      CP2(N)=ASG(N)*GK(N)*(P2(N)*D2(N)+P3(N)-1.0)
000111      PK1,NDX1+1) = PC021
000112      PK2,NDX1+1) = PH201
000113      DO 26 N=1,NDX1
000114      N1=NDX1+1-N
000115      I=IFN(N1,NDXM)
000116      PK1,N1) = (PK(1,N1+1)/DX+CP1(N1)/A(N1))
000117      1/(1./DX-CP2(N1)/A(N1))
000118      IF (I.EQ.1) J=2

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000119 IF(1.EQ.2)J=1
000120 PK(J,N1)=PK(J,N1+1)
000121 CONTINUE
000122
000123
000124 C TO CALCULATE SORBENT LOADING
000125 C
000126 C DO 30 N=1,NDXM
000127 C I=IFN(N,NDXM)
000128 C W(NDR4,N)=Q(NDR4,N)+D2(N)*PK(1,N)
000129 C DO 30 J=2,NDR4
000130 C L=NDR4+1-J
000131 C 3C W(L,N)=Q(L,N)*B(L,N)*W(L+1,N)
000132
000133 C
000134 C IF( NTEMP .EQ. 0) RETURN
000135 C TO CALCULATE SORBENT, GLYCOL, HX CORE AND GAS TEMPERATURES
000136 C
000137 C CALL TSCRBA
000138 C CALL TGLCOL(TC,NDX1,UC,RHOC,CPC,CX,AXC,HXC,T268,TX,DX,DT,AVC,NOG)
000139 C CALL HXCORE(TX,TC,TS,TG,HAC,HXS,HXG,RHOX,CPPX,TRX,DX,DT,NDX1,AVX,
000140 C 1NDXM)
000141 C CALL GASTA(GMR,CPG,ABED,NDX1,TG1,ASC,HSG,AXG,HXG,DX,TG,TS,TX)
000142 C RETURN
000143 C
000144

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• ELT 59970-1, 690501, 43763

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000001      SUBROUTINE CASTG(CMR,CPC,ABED,NDX1,TG1,ASC,HSG,AXC,DX,TG,TS,TX
000002
000003      C
000004      C   GAS TEMPERATURE CALCULATIONS FOR ADSORPTION
000005      C
000006      DIMENSION CPC(1),ASG(1),HSG(1),HXC(1),TG(1),TS(1),TX(1),ABED(1),
000007      JAXG(1)
000008      C
000009      TG(NDX1+1) = TG1
000010      DO 10 N=1,NDX1
000011      N1=NDX1+1-N
000012      CGMRO=P(G(N1)/ABED(N1)
000013      C1=ASC(N1)*HSG(N1)+AXG(N1)*HXC(N1)
000014      10  TG(N1) = (TG(N1+1)/DX*(ASG(N1)*HSG(N1)*TS(N1)+AXG(N1)
000015      *HXC(N1)*TX(N1))/
000016      1C)/(1./DX*C1/C)
000017      RETURN
000018      END

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• ELT-99977, 1, 690501, 43784

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000001
000002
000003
000004
000005      SUBROUTINE TSORBA
COMMON /BLOK2/ ABED(41), A(41), AVG(41), CPG(41), RHOG(41),
1HGX(41), HXS(41), HXC(41), DTF(41), F(41), C(41), VS(2), DVS1(2), R
000006          2S1(2,41), RHOS(2), UG(41), WML2, UC(41), NDXM, PS(41), RHOSB(41), DS(41),
000007          3CS1(41), CS2(41), C1(21,41), C2(21,41), D1(21,41), D2(41), PC1(41), PC2(4
000008          41), PC3(41), ASG(41), ASX(41), AGX(41), C1P(41), C2P(41), C3P(41), D1P(41)
000009          5, FR(2,41), RS(2), NDX1, NDR4, DX, DT, GK(41), DH(41), SK(41), P1(41), P2(41)
000010          6, P3(41), WS(41), CR(12,21), CR2(2,21), CR3(2,21), C1(21,41), C2(21,41),
000011          7Q(21,41), CP1(41), CP2(41), X(41), VOID(41), TIME
000012          A, AXCL(41), RHOC(41), CPC1(41), T268, AVX(41), JKX(41), CPX(41),
000013          9, NOC, PK(2,41), PCO21, PH201, GMR, GMW, TCI, PA, PT(41), CPS(41), MSG(41)
000014
000015      COMMON /BLOK3/, Y(21,41), TC(41), TX(41), CYCLE
000016      DOUBLE PRECISION W
000017      COMMON /BLOKA/ D10, TS1(41), TS2(41), TX1(41), TX2(41), TC1(41), TC2(41)
000018      DIMENSION S1(41), S2(41), SJ(41), BI(41)
000019      DO 10 N41, NDX1
10      T2(DT,DT)/CPS(N)/RHOSB(N)
1A3D  2.0*TS(AGC(N)*MSG(N)*ASX(N)*HXS(N))
000021
000022      CS1(N)=CS1(N)(1,0,T1)
000023      CS2(N)=CS2(N)(1,0,T1)
000024      11FN(N,NDXM)
000025      IGAMC1(SIGL,N)
000026      B1(N)=TS2(N)*CS1(N)*
000027      1PKL1(N)
000028      2
000029      1P1(N)*
000030      2PK(1,N)
000031      2
000032      4ASX(N)*HXS(N)*TX1(N)-T1*TS2(N)
000033      1FIN, EQ, 1)  S1(N)=0,0
000034      IF(N, EQ, 1)  GO TO 11
000035      S1(N)=1-FSK(N)/DX/DX*ABED(N-1)*ABED(N)/(2.*ABED(N))
000036      11 S2(N)=7*SK(N+1)/DX/DX*(ABED(N)+ABED(N+1))/12.*ABED(N)
000037      S2(N)=S1(N)-S3(N)+T1
000038      10 CONTINUE
000039      CALL FDE01M(S1,S2,S3,R1,T5,NDX1)
000040      RETURN
000041

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SUBROUTINE STARTA
C
COMMON /BLOK2/ ABED(41), A(41), AV(41), CPG(41), RHOC(41),
1HXC(41), HXS(41), HYC(41), HYD(41), VS(2), DV81(2), R
2S1(2,1), RHOS(2), UG(41), WM(2), UC(41), NDHM, RS1(41), RHOSB(41), DS(41),
3CS1(41), CS2(41), C1(21,41), C2(21,41), D1(21,41), D2(41), PC1(41), PC2(4
41)+PC3(41), ASC(41), ASX(41), CIP(41)+C2P(41)+C3P(41)+D4P(41),
5,FR(2,41), RS(2,NDX1,NDX1), DX, DT, DK(41), DH(41), SK(41), P1(41), P2(41),
6,P1(41), WS(41), CR1(2,21), CR2(2,21), CR3(2,21), C3(21,41), B(21,41),
7Q(21,41), CP1(41), CP2(41), X(41), V0DF(41), TIME
8,AXC(1,1), RHOC(41), CPC(1,1), TX(41), RX(41),
9,NOG,PK(2,41), PC02(1, PHZ01), GMR, GMW, TGL, PA, PT(41), OPS(41), HSG(41)
--COMMON /BLOK3/ N(21,41), TC(41), TS(41), IC(41), TX(41), CYCLE
--DOUBLE PRECISION W
DO 115 N=1,NDX1
115 A(N)= GMR/ABED(N)/PA/GMW
C
C
RS(1,1)*RHOSB(1,1),/RS(1,1)/ASC(1)
RS(2,1)*RHOSB(NDX1)
1
NDR=NDR4-1
NDR2=2*NDR
NDR3=NDR2+1
DO 10 L=1,2
V$1(1)*4./3.*3.14159*RS(1)*0.03
DV5(1)*DV5(1)/ADR
DV5(1)=DV5(1)/2.
RS1(1,1)=0,
DO 10 K=2,NDR3
10 RS1(1,1)=K*3.14159514./3.*3.14159514.*K,4.14159514.*K,4.14159514.*K
DO 11 I=1,2
1E1,I,E0,1) DIF1*DIF(1)
IF (I, EQ, 2) DIF1*DIF(NDX1)
CR1(1,1)=DV5(1)*RHOS(1)
CR1(1,1)=3.14159*RS1(1,2*K-2)*2*DIF1 /(RS1(1,2*K-1)-RS1(1,2*K))
13) *RHOS(1)
11 CR3(1,1)=3.14159*RS1(1,2*K)*2*DIF1 /(RS1(1,2*K+1)-RS1(1,2*K-1)
1) *RHOS(1)
CR1(1,1)=CR1(1,1)
CR1(2,1)=CR1(2,1)
END

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SUBROUTINE PRADS

```

000001      C
000002      C
000003      C
000004      DIMENSION AVLD(41), AVC(41), CPG(41), RHOG(41),
000005      COMMON /BL0K2/ ABED(41), A(41), AVC(41), C(41),
000006      1HXC(41), HXS(41), HYC(41), DIF(41), F(41), G(41),
000007      2S12.4,1.,BHOSB(2),UC(41),NDXM,PS(41),RHOSB(1),DS(41),
000008      3CS1(41)CS2(41)C1(21,41)C2(21,41)D1(21,41)D2(41)PC1(41)PC2(4
000009      41)PC3(41)ASC(41)ASX(41)GK(41)CP(41)C1B(41)D1P(41)
000010      5,F(2,41),RS(2),NDY1,NDR4,DV,DT,GK(41),DH(41),SK(41),P1(41),P2(41)
000011      6,P3(41),HS(41),CR(2,21),CR2(2,21),CR3(2,21),C3(21,41),B(21,41),
000012      70(21,41),CP1(41),CP2(41),X(41),VO,DF(41),TIME
000013      B,AXC(41),RHOC(41),CPG(41),CPX(41),RHDX(41),
000014      9,NOG,PK(2,41),PC021,PH201, GMR,GMW,TG,PA,PT(41),CPS(41),HSG(41)
000015      COMMON /BL0K3/ W(21,41),TC(41),TS(41),TX(41),CYCLE
000016      DOUBLE PRECISION W
000017      COMMON /BL0K4/ POUT(10),TINET(10),NBOUT,NPSET(3)
000018      COMMON /BL0K5/ NCCLT
000019      COMMON /BL0K6/ DTD,TS1(41),TS2(41),TX1(41),TX2(41),TC1(41)+TC2(41)
000020      COMMON /BL0K10/ NPRINT,DTMAX,NOTCON
000021      COMMON /BL0K11/ TOTCO2,TOTHO2,SUMPTM,WTACMS,W,SG
000022      COMMON /BL0K12/ NTEMP
000023      COMMON /BL0K13/ NI, TI
000024      COMMON /BL0K14/ NCYCLE
000025      COMMON /BL0K15/ NDXMAC, PC025, VOLCAB, RC02C
000026      COMMON /BL0K17/ NSTART
000027      DIMENSION AXS(41),AXG(41),AGS(41),HGX(41),HGS(41),ACX(41),
000028      1HCX(41)
000029      EQUIVALENCE (AXS,AXS),(ACX,AXG),(ASG,AGS),(HGX,MSX),(HGS
000030      1,MS),(ACX,ACX),(HGX,HGX)
000031      EQUIVALENCE (NDX,NDX1)
000032      APWH20 = SUMPTM/TIME
000033      APWH20=GHRAVPH2010./(PA*GMW)
000034      C
000035      TIME=6D.0,TIME, TIME, TIME, DT
000036      WRITE (6,100) NCYCLE, TIME, TIME, DT
000037      WRITE (6,101)
000038      WRITE (6,102)(N,PK1,N),PK(2,N),
000039      1,          TG(N),TS(N),TC(N),TX(N),N=1,NDX
000040      WRITE (6,202)
000041      N1=NDXMH1,
000042      NDJ3=NDR4+1
000043      DO 20,NE=1, NDXM
000044      SUMMS=0.0
000045      SUMMS=SUMMS+0.5*(W(1,N)+W(NDR4,N))
000046      IF(NDR4.EQ.2) AVLD(N)=SUMMS
000047      IF(NDR4.EQ.2) GO TO 20
000048      DO 22 NR=2,NDR3
000049      22 SUMMS=SUMMS+W(NR,N)
000050      AVLD(N)=SUMMS/NDR3
000051      20 CONTINUE
000052      DO 30 NF=N1,NDX1
000053      SUMMS=0.0
000054      SUMMS=SUMMS+0.5*(W(1,N)+W(NDR4,N))
000055      IF(NDR4.EQ.2) AVLD(N)=SUMMS
000056      IF(NDR4.EQ.2) GO TO 30
000057      DO 33 NR=2, ND'R3
000058      33 SUMMS=SUMMS+W(NR,N)

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000059      AVLD(N)*SUMMXS/ANDR3
000060      30 CONTINUE
000061      SUM=0
000062      IF(NDXMAC .EQ. 0) GO TO 35
000063      DO 31 N= 1, NDIMAC
000064      31 SUM= SUM+AVLD(N)*ABED(N)*DX*RHOSS(N)
000065      AVMSLD = SUM*WTACMS
000066      SUM=0
000067      -35 CONTINUE
000068      IF((NDX1-NDXM) .EQ. 0) GO TO 40
000069      DO 32 NR=N1,NDX1
000070      32 SUM = SUM+AVLD(N)*ABED(N)*DX*RHOSS(N)
000071      AVGSLD=SUM/WTSG
000072      40 CONTINUE
000073      DO 10 NR=1,NDX
000074      10 WRITE (6,203) NR, AVLD(N)
000075      1      4 (NR,NR,NR,NR)
000076      WRITE (6,205) AVMSLD, AVGSLD
000077      AVRCO2=TOTCO2/VTIME
000078      AVRH2=10TH20/VTIME
000079      WRITE(6,204) AVRCO2,AVRH20
000080      WRITE(6, 206) AVPH20, AVH20P
000081      RETURN
000082      100 FORMAT (1H1,16HADSORPTION CYCLE, 13/
000083      1      3X,5H TIMES, F9.3,1X2WHR,F12.3-1X,1MMIN,
000084      1      5X,1SWTIME,F9.3,1X2WHR,F12.3-1X,1MMIN,
000085      1      101 FORMAT (//2X,10HAXIAL NODE,1X,2WCO2,MM,5X,2WPM20,MM,AX,
000086      1      1      6X,15WBORENT-TEMP, F- ,6X,15WCOOLANT-TEMP, F- ,7X,15WHX,CO.
000087      1      2RE TEMP, F )
000088      102 FORMAT (//19,2E12.4,5X,(E14.4,6X))
000089      103 FORMAT (//38HLOADING AT INTERIOR OF SOBENT, LBLB
000090      1      1      15,4X,12(F6.4,1X))
000091      1      1      1E,3X, 3HVG, 9X,
000092      1      1      1H1.9X,1H2.9X,1M3.9X,1M4.9X,1M5.9X,1M6.9X,1M7.9X,
000093      1      21H8.9X,1H9.8X,2H10,
000094      1      28X,2A11/6W AXIAL/5H NODEB)
000095      203 FORMAT ( 15,4X,12(F6.4,1X))
000096      204 FORMAT (//22HDTIME AVG-CO2 ADSORP RATE, F )
000097      205 FORMAT (//,20H AVG CO2 LOADING IN M.S. BED, F8.4, 6W LB/LB)
000098      1      F8.4, 6W LB/MR ,10X
000099      1      227H TIME AVG-LB20 ADSORP RATE, F )
000100      1      3 F8.4, 7W LB/MR
000101      1      206 FORMAT (//,20H AVG H20 LOADING IN S.G. BED = F8.4, 6W LB/LB)
000102      1      130H AVG H20 LOADING IN S.G. BED = F8.4, 6W LB/LB
000103      1      206 FORMAT (//,21H TIME AVG EXIT PL20, F10.4, 1H MM,10X,
000104      1      140H TIME AVG RATE OF M.S. POISONING BY H20 = , G12, 6,10W LB M20/LB)
000105      END

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0000001      C   SUBROUTINE MODEOR FOR TRANSIENT DESORPTION BED CALCULATIONS
0000002      C
0000003      C
0000004      C   COMMON /BLOK1/ ABED(41), A(41), AVG(41), CPG(41), RHOC(41),
0000005      C   1HGX(41), HXS(41), HXC(41), E(41), C(41), DIF(41), VS(2), DVS(2), R
0000006      C   2S1(2,41), RMOS(2), UG(41), UC(41), W(2), UC(41), RMOSB(41), DS(41),
0000007      C   JCS1(41), CS2(41), C1(21+41), C2(21+41), D1(21+41), PC1(41), PC2(4
0000008      C   41), PC1(41), ASG(41), ASX(41), AGX(41), CIP(41), CIP(41), DIP(41)
0000009      C   5, ER(2,41), RS(2,41), NDR4, DX, DT, GK(41), DH(41), SK(41), P1(41), P2(41),
0000010      C   6, P3(41), WS(41), CR1(2,21), CR2(2,21), CR3(2,21), C3(21,41), B(21,41),
0000011      C   7Q(21,41), CP1(41), CP2(41), X(41), VD1DP(41), TIME
0000012      C   8, AXC(41), RHOC(41), CPC(41), T268, AVX(41), TKX(41), CPX(41), RHOX(41)
0000013      C   9, NDC, PK2, A11, PCG21, PH2Q1, QMR, GMH, IGL, PA, P1(41), CPS(41), MSG(41).
0000014      C   DOUBLE PRECISION C1, C2, D1, D2, PC1, PC2, PC3, P1, P2, P3, C3, G, B,
0000015      C   1, C4, CP3, CP2, X, DI
0000016      C   DOUBLE PRECISION C1P, C2P, CSP, D1P
0000017      C   COMMON /BLOK3/ H(21,41), T(41), TS(41), TC(41), TX(41), CYCLE
0000018      C   DOUBLE PRECISION W
0000019      C   COMMON /BLOK8/ DIO, IS1(41), IS2(41), IX1(41), IX2(41), TC1(41), TC2(41)
0000020      C   COMMON /BLOK10/ NPRINT, DMAX, NDTCON
0000021      C   COMMON /BLOK11/ TOTC02, TOTH20
0000022      C   COMMON /BLOK12/ WI, TI
0000023      C   COMMON /BLOK14/ NCYCLE
0000024      C   COMMON /BLOK17/ NSTART
0000025      C
0000026      C   TIME = 0.0
0000027      C   DIO = 50.0
0000028      C   DT=1.E-5
0000029      C   TOTC02=0.0
0000030      C   TOTH20=0.0
0000031      C   DO 20 N=1,NDX1
0000032      C   TS1(N)= TS(N)
0000033      C   TS2(N)= TS(N)
0000034      C   TX2(N)=TX(N)
0000035      C   TX1(N)=TX(N)
0000036      C   TC1(N)=TC(N)
0000037      C   IC2(N)=TC(N)
0000038      C   20 CONTINUE
0000039      C   IF TIME .GE. CYCLE) GO TO 9999
0000040      C   CALL PRD68
0000041      C   NPI = 0
0000042      C   GO TO 3
0000043      C   2 CALL PRD68A
0000044      C   IF TIME .GE. CYCLE) GO TO 9999
0000045      C   CALL START
0000046      C   NPI = 0
0000047      C   4 CONTINUE
0000048      C   DTO=DT
0000049      C   GO TO (41,42), NDTCON
0000050      C   41 ADI=DTHMAX
0000051      C   DO 60 N=1,NDX1
0000052      C   ADT2=W1 - /ABS(W(NDR4,N)*WS(N))+1,E-9)/DT
0000053      C   IF(ADT2.LT. ADT) ADT=ADT2
0000054      C   ADI2=T1/(ABS1(.IS(N)-TS2(N))+1.E-9)*DT*2.0
0000055      C   1F(ADT2.LT. ADT) ADT=ADT2
0000056      C   ADT2=S1L((ABS(-IX(N)-TX2(N))+1.E-9)*DT*2.0
0000057      C   1F(ADT2.LT. ADT) ADT=ADT2
0000058      C   ADI2=T1/((ABS( TC(N)-TC2(N))+1.E-9)*DT*2.0
0000059      C   IF(ADT2.LT. ADT) ADT=ADT2

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000059   60 CONTINUE
000060   DT=DT
000061   GO TO 3
000062   42 DT=DYMAX/10.0
          IF(TIME .LT. 1.E-4) DT=DTMAX/1000.0
          IF(TIME .GT. 0.06) DT=DYMAX
000063   3 CONTINUE
          IF((TIME+DT) .GT. CYCLE) DT = CYCLE-TIME
          DO 21 N=1,NDX1
              TS2(N)=TS1(N)
              TS1(N)=TS(N)
              TX2(N)=TX1(N)
              TX1(N)=TX(N)
              TC2(N)=TC1(N)
              TC1(N)=TC(N)
21      CONTINUE
000069   D9DT
000070   CALL DESORB(0)
000071   TOTCO2=TOTCO2+DT*FR(1,NDX1)*NM(1)
000072   TOTH2=TOTH2+DT*FR(2,NDX1)*WM(2)
000073   TIME=TIME+DT
000074   NPRINT+1
000075   IFL_(NPR,GE,NPRINT),AND,(NCYCLE,GE,INSTANT)) GO TO 2
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000077   000078
000078   000079
000079   000080
000080   000081
000081   000082
000082   000083
000083   000084
000084   000085
000085   9999 CONTINUE
          RETURN
000086   END

```



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```
FUNCTION IFN(N,NDXM)
IFN=1
IF(N,GT,NDXM)IFN=2
RETURN
END
```

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000003
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DO 12 N=1,NDX1
 1=IFN(N,NDXH)
  CS2(N)=DT/CPS(N)/RHOS3(N)*ASG(N)*GK(N)*WM(1)*DH(N)
  CS1(N)=CS2(1)*X(N)
  IF(N.EQ.1) S1=((ABED(N)+ABED(N+1))*SK(N+1)*(TS(N+1)-TS(N)))/(2.*ABED(N)*UXDX)
  1 ABED(N)*UXDX
  1 IF(N.EQ.1) GO TO 15
  S1=((ABED(N-1)+ABED(N))*SK(N)*(TS(N-1)-TS(N))+ABED(N)*ABED(N+1))
  1 *SK(N-1)*(TS(N+1)-TS(N)))/(2.*ABED(N)*DX*DX)
  1 DS(N)=DT/CPS(1)/(RHOS3(N)*(SI+ASG(N)*HSG(N)*(TG(N)-0.5*TS2(N))+IASX(N)*HXS(N)*(TX(N)-0.5*TS2(N)))
  RATIO=(DT-DT0)/DT
  T=(DT+DT0)/CPS(N)/(RHOSB(N))
  T1=0.5*T*(ASC(N)*HSG(V)+ASX(N)*HXS(N))
  CS1(N)=RATIO*CS1(N)/1.+T1)
  CS2(N)=RATIO*CS2(N)/(1.+T1)
  DS10=DS(N)
  DS(N)=RAT10*DS(N)
  DS(N)=(DS(N)-T1*TS2(N))/(1.+T1)
  12 CONTINUE
  GO TO 110
  111 DO 112 N=1,NDX1
    CS1(N)=0.
    CS2(N)=0.
    DS(N)=0.
    TS(N)=T268
    TC(N)=T268
    TX(N)=T268
    TG(N)=T268
    112 CONTINUE
    110 CONTINUE
  C TO CALCULATE TOTAL PRESSURE
  C
  DO 24 N=1,NDX1
    1=IFN(N,NDXH)
    TO CALCULATE P1,P2,P3
    WSURF=W(NDR4,N)
    PSURF=PKEQ1(WSURF,TS2(N))
    DPKDTS=PKEQ1(WSURF,TS2(N))
    1/ (PKEQ1(WSURF,(TS2(N)+0.001))-PSURF
    20.001 DPKDWK=(PKEQ1(WSURF+1.E-6),TS2(N))-PSURF
    1.E-6 G=1.+CS2(N)*DPKDTS
    P1(N)=(PSURF+DS(N)*DPKDTS)/G
    P2(N)=DPKDWS/G
    P3(N)=CS1(N)/G*DPKDTS
  C
    C2(NDR4,N)=CR1(1,NDR4)/DT+CR2(1,NDR4)+WM(1)*GK(N)*P2(N)*AS(1)
    C3(NDR4,N)=0.0
    DO 23 NR=1,NDR4
      D1(NR,N)=CR1(1,NR)/DT*W(NR,N)
      D1(NDR4,N)=D1(NDR4,N)-WM(1)*GK(N)*(P1(N)-P2(N))*W(NDR4,N)*AS(1)
      D2(N)=AS(1)*H(1)*GK(V)*(X(N)-P3(N))
      D2(N)=D2(N)/C2(NDR4,V)-C1(NDR4,N)*B(NDR4-1,N)
      Q1(1,N)=D1(1,N)/C2(1,N)
      DO 24 J=2,NUR4
        Q(J,N)=(D1(J,N)-C1(J,V)*Q(J-1,N))/(C2(J,N)-C1(J,N)*B(J-1,N))
  24 Q(J,N)=(D1(J,N)-C1(J,V)*Q(J-1,N))/(C2(J,N)-C1(J,N)*B(J-1,N))
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000119
000120      DO 25 N=2,NDX
000120      25 PC2(N)=PT(N)/(VOIDF(N)*C(N)*ABED(N))*(VOIDF(N+1)*C(N+1)*ABED(N+1)
000121      1)/F(N-1) - VOIDF(N-1)*C(N-1)*ABED(N-1)/F(N-1)/(2.*DX)
000122      N=1
000123      PC2(N)= PT(N)/(VOIDF(N)*C(N)*ABED(N))*(VOIDF(N+1)*C(N+1)*ABED(N+1)
000124      1)/F(N-1) - VOIDF(N )*C(N )*ABED(N )/F(N )/(1.*DX)
000125      N= NDX1
000125      PC2(N)= PT(N)/(VOIDF(N)*C(N)*ABED(N))*(VOIDF(N )*C(N )*ABED(N )
000126      1)/F(N ) - VOIDF(N-1)*C(N-1)*ABED(N-1)/F(N-1)/(1.*DX)
000127      DO 26 N=1,NDX1
000128      PC1(N)=PT(N)/F(N)
000129      PC1(N)=PT(N)/F(N)
000130      PC3(N)=PT(N)/C(N)/VOIDF(N)*GK(N)
000131      C
000132      DO 27 N=1,NDX1
000133      CP1(N)=PC3(N)*P1(N)+2*(N)*(NDR4,N)-W(NDR4,N))
000134      CP2(N)=PC3(N)*P2(N)+2*(N)+P3(N)
000135      C1P(N)=-PC1(N)*DX+PC2(N)/2./DX
000136      C2P(N)=1./DT+2.*PC1(N)*DX+PC2(N)/2./DX
000137      C3P(N)=-PC1(N)*DX/DX-PC2(N)/2./DX
000138      D1P(N)=PT(N)/DT+CP1(N)
000139      C
000140      C  BOUNDARY CONDITION FOR P-EQUATION
000141      C2P(1)=C2P(1)*C1P(1)
000142      C1P(1)=0.
000143      GO TO (55,56), NBCOUT
000144      55 CONTINUE
000145      PTNDX1=PT(NDX1)/0.888
000146      CEX1=(ALOG(PThDX1)+1.76)/(1.96*PT(NDX1))/(VOIDF(NDX1)*RHOG(NDX1)
000147      1.*ABED(NDX1))
000148      C2P(NDX1)= C2P(NDX1)+C3P(NDX1)*(1.-DX*F(NDX1)*CEXT)
000149      C3P(NDX1)=0.0
000150      GO TO 57
000151      56 CONTINUE
000152      C  PRESSURES ARE SET
000153      C
000154      50 561 K= 1, 3
000155      IF (NPSET(K) .EQ. 0) GO TO 561
000156      NP=NPSET(K)
000157      C1P(NP)=0.0
000158      C2P(NP)=1.0
000159      C3P(NP)=0.0
000160      CALL LAGIN2(10,TIMET,10,2,TIMF,D1PNP ,POINT)
000161      D1P(NP)=D1P*P
000162      561 CONTINUE
000163      57 CONTINUE
000164      CALL FDEGID(C1P,C2P,C3P,D1P,PD,NDX1)
000165      DO 34 N=1,NDX1
000166      IF (PD(N) .LE. 0.) PD(N) = 1.E-3
000167      34 PT(N)=PD(N)
000168      C  TO CALCULATE SORBENT LOADING
000169      00 30 N=1,NDX1
000170      W(NDR4,N)=Q(NDR4,N)+D2(N)*PT(N)
000171      DO 30 J=2,NUR4
000172      000173      L=NDR4+1-J
000173      000174      W(L,N)=Q(L,N)-B(L,N)*W(L+1,N)
000175      000176      C  TO CALCULATE STREAM COMPOSITION
000176      000177
000177

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```

C      FR(1,1) = 0.0
000160
000181
000182
000183      FR(2,1)=0,
000184      DO 31 N=1,NDX1
000185      I=IFN(N,NDX1)
000186      TEMP =C(N)*VOIDF(N)
000187      1/P4(N)*ABED(N)
000188      IF(I,EQ,1)J=2
000189      IF(I,EQ,2)J=1
000190      IF(N,EO,1) GO TO 200
000191      FRC(J,N)=FRC(J,N-1)
000192      FR(1,N)=TEMP+FR(1,N-1)
000193      IF( NDXM, EQ, 0) GO TO 202
000194      IF (I,EQ,1) GO TO 202
000195      IF( NPS(2), IE, 0) GO TO 202
000196      GO TO 201
000197      200 FR(1,1) = TEMP
000198      202 X(N) = 1.0
000199      GO TO 31
000200      201 CONTINUE
000201      CT=ABED(N)*DX*ASG(N)*GK(N)
000202      FRT= FR(1,N)+R(2,N)+1.E-10
000203      PSURF = P1(N)*P2(N)*(VNDR4,N)-WS(N)*P3(N)*PT(N)
000204      X(N)=(FR(2,N-1)+CT*PSURF
000205      1*(1+CT*PT(N)*FRT))
000206      IF(X(N)) .LT. 0.0 X(N)=0.0
000207      IF(X(N)) .GT. 1.0 X(N)=1.0
000208      31 CONTINUE
000209      DO 33 N=1,NDX1
000210      C(N) =(PT(N))/RGAS/(TG(N)+460)+C(N))/2.0
000211      I = IFN(N,NDM)
000212      IF (I,EO,1) J=2
000213      IF (I,EG,2) J=1
000214      RHOG(N)=C(N)*X(N)*WM(1)+(1.-X(N))*WM(J)
000215      UG(N)=(FR
000216      1,(1.,)WM(1)+FR(2,N)*WH(2))/RHOG(N)/ABED(N)/VOIDF(N)
000217      33 CONTINUE
000218      IF( NTEMP, EQ, 0) RETURN
000219      C      TO CALCULATE SORBENT TEMPERATURES
000220      CALL TSRRB
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* ELT 59904,1,690901, 43794

```
000001      SUBROUTINE FDEQM(C1,C2,C3,Q,VAR,NN)
000002          DIMENSION C1(1),C2(1),C3(1),Q(1),VAR(1),B(41),O(41)
000003          NN1=NN-1
000004          B(1)=C3(1)/C2(1)
000005          DO 41 J=2,NN1
000006          41   B(J)=C3(J)/(C2(J)-C1(J)*B(J-1))
000007          Q(1)=O(1)/C2(1)
000008          DO 42 J=2,NN
000009          42   Q(J)=D(J)-C1(J)*Q(J-1)/(C2(J)-C1(J)*B(J-1))
000010          VAR(NN)=Q(NN)
000011          DO 43 J=2,NN
000012          43   L=NN+1-J
000013          VAR(L)=Q(L)-B(L)*VAR(L+1)
000014          RETURN
000015          END
```

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• ELI-S90A5.1.690501, 43795

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000001      SUBROUTINE FDEQD(C1,C2,C3,D,VAR,NN)
000002      DIMENSION C1(1),C2(1),C3(1),D(1),VAR(1),B(41),Q(41),
000003      DOUBLE PRECISION C1,C2,C3,D,VAR,B,Q,
000004      NN1=NN-1
000005      B(1)=C3(1)/C2(1),
000006      DO 41 J=2,NN1
000007      A1=B(CJ)*C3(CJ)/(C2(CJ))-C1(CJ)*B(CJ-1)
000008      Q(1)=B(1)/C2(1),
000009      DO 42 J=2,NN
000010      Q(1)=((Q(1)-C1(J)*B(J-1))/(C2(J)-C1(J))*B(J+1))
000011      VAR(NN)=B(NN)
000012      DO 43 J=2,NN
000013      L=NN+1-J
000014      43  VAR(L)=Q(L)-B(L)*VAR(L+1)
000015      RETURN
000016

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• ELLI 59986.1.690501, 43796

```

000001      SUBROUTINE GAST_(DX,RHOG,CPQ,U,TS,TX,NDX1,ASG,HSG,AHG,TG,VOIDF
000002      1)
000003      DIMENSION RHOG(1),CPQ(1),U(1),TS(1),TX(1),TG(1),AG(1),HSG(1),AHG(
000004      11),VOIDF(1),ASG(1),
000005      N1=1,Q
000006      N2= NDX1-1
000007      TG(1)=TS(1)
000008      DO 10 N = 1, N2
000009      EP 0.5*(VOIDF(N)* VOIDF(N+1))
000010      AS1=ASG(N+1)
000011      HS1=HSG(N+1)
000012      AX1=AG(N+1)
000013      HX1=AHG(N+1)
000014      CP1=CPQ(N)
000015      RO=.4 D.5*(RHOG(N)*RHOG(N+1))
000016      U1= 0.5*( U(N)+U(N+1))
000017      TS1=S(N+1)
000018      TX1=X(N+1)
000019      C1M1./((F=R0*CP1*U1)
000020      D4C1=(AS1*HS1)*TX1*AX1*TX1)
000021      A=(AS1*HS1*AHG(HX1))*C1
000022      10 TG(N1)=((1./DX-A(1,-1))*TD(N))D/(1./DX*A(0,W))
000023      RETURN
000024      END

```

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ELI 59967, 11090204, 43797

```

SUBROUTINE TGLCOL(TC,NDXMAX,UC,RHOC,CPC,CX,AXC,HXC,T268,TX,DX,DT,
 1AVC, NOGLIN)
 000002 DIMENSION C1(41),C2(41),C3(41),D(41),TC(1),TX(1),HXC(1),AVC(1),B(4
 000003 11),Q(41),
 000004 000005 DIMENSION UC(11),RHOC(11),CPC(11),AXC(11)
 000006 COMMON /BL0K8/,DT0,TS1(41),TS2(41),TC1(41),TC2(41)
 000007 ONEDT*DT0
 000008 DO 10 N=NOGLIN,NDXMAX
 000009 C01=UC(N)
 000010 CC2=HXC(N)/(CPC(N)*RHOC(N))*AVC(N)*0.9
 000011 IF( UC(N) < GT, 0.1 GO TO 9
 000012 C3(N)=CC1/DX
 000013 C2(N)=1./DN+CC2*C3(N)
 000014 C1(N)=0.0
 000015 GO TO 10
 000016 5 C1(N)= CC1/DX
 000017 C2(N)= -1./DN + CC2 * C1(N)
 000018 C3(N)= 0.0
 000019 10 DN1=TC2(N)/DN*CC2*TX1(N)+2.*CC2*TC21(N)
 000020 C1(NOGLIN)=0.
 000021 C1(NOGLIN)= Q.
 000022 D(NOGLIN)=D(NOGLIN)+AB8(UC(NOGLIN))/DX*T268
 000023 NOG2=NOGLIN-1
 000024 DO 51 N= 1, NOG2
 000025 51 TC1=N*0.00
 000026 NNN=NOGLIN
 000027 NN1=NN-1
 000028 N1=NOGLIN
 000029 N2=NN1+1
 000030 B(N1)=C3(N1)/C2(N1)
 000031 DO 41 JEN2>NN1
 000032 41 B(J)=C3(J)/C2(J)-C1(J)*B(J-1)
 000033 Q(N1)=D(N1)/C2(N1)
 000034 DO 42 J=N2,NDXMAX
 000035 42 Q(J)=(D(J)-C1(J)*Q(J-1))/(C2(J)-C1(J)*B(J-1))
 000036 TC(NN)=Q(NN)
 000037 DO 43 J=NN-1,NN
 000038 43 L=NN+N1-J
 000039 TC(L)=Q(L)-B(L)*TC(L+1)
 000040 RETURN
 000041 END

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• ELT 6998A-1490617, 53903

SUBROUTINE_START

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000001      C
000002      COMMON /BLOK1/ ABED(41), A(41), AVCT(41), CPG(41), RHOC(41),
000003          HXC(41), HXS(41), HVC(41), DIF(41), F(41), C(41), VS(2), DV51(2), R
000004          2S1(2), UC(41), NDXM, PS1(1), RDOSB(1), DS(41),
000005          CS1(41), CS2(41), C1(21,41), C2(21,41), D1(21,41), D2(41), PC(4
000006          11), RC1(1), ASGL(1), ASX(41), AGX(41), C2P(41), C2P1(41), C2P1A(1), D1P1A(1)
000007
000008          S, PR(2,41), RS(2), NDX1, NDRA, DX, DT, GK(41), DH(41), SM(41), PI(41), P2(41)
000009          A, PI(41), WS(41), CR1(2,21), CR2(2,21), RS(2,21), C3(21,41), B(21,41),
000010          T0(21,41), CP1(41), CP2(41), X(41), VO1DF(41), TIME
000011          S, AXC(41), RHOC(41), CPG(41), TXK(41), TXK(41), TXK(41),
000012          9, NOG, PK(2,41), PC021, PW201, GMR, GMW, TG1, PA, PT(41), CPS(1), HSC(41)
000013          DOUBLE PRECISION C1, C2, D1, D2, PC1, PC2, PC3, R1, R2, P1, C3, Q, B,
000014          1, CP1, CP2, X, DT
000015          1, DOUBLE PRECISION C1P, C2P, C3P, D1P
000016          COMMON /BLOK3/ W(21,41), TC(41), TS(41), TX(41), CYCLE
000017          DOUBLE PRECISION W
000018
000019          IS1(NDXM) = NDXM
000020          DMF = 0, 0, 157
000021          RS(1) = RHOSB(1), ARG(1)
000022          RS(2) = RHOSB(NDXM)
000023          1, 0, 1, /RHOSB(2), ARG(NDXM)
000024          DO 30 N = 1, NDX1
000025          RHOSB(N) = 0, 0001
          X(N) = 1, 0
000026          10, IF(NN, NDXM)
000027          15, NN = NDXM
000028          15, NN = NDXM
000029          1E(1D, EQ, 2), X(N) = S + DMF
000030          C(2) = 0, 2E-3
000031          P(1) = 6, 00
000032          1, IF(NN, NDXM)
000033          10, VOIDFN, S - 1, * RHOSB(N) / RHOSB(1)
          X(NDXM+1) = 0, 01
000034          NDR = NDRE = 1
000035          NDR2 = 2, NDR
000036          NDR3 = NDR2 + 1
000037          DO 10 K = 2, NDR3
000038          10, RS1(1, K) = CBRT(3, /4, /3, 1416*RS(1)) + 3*DVS1(1)
000039          V(1) = 3, *3, *3, 1416*RS(1) + 3
000040          DVS(1) = VS(1) / NDR
000041          DVS1(1) = DVS(1) / 2
000042          RS1(1, 1) = 0,
000043          DO 10 K = 2, NDR3
000044          10, RS1(1, K) = CBRT(3, /4, /3, 1416*RS(1, K-1)) + 3*DVS1(1)
000045          10, RS1(1, 1) = 0,
000046          10, RS1(1, K) = CBRT(3, /4, /3, 1416*RS(1, K-1)) + 3*DVS1(1)
000047          10, RS1(1, 1) = 0,
000048          10, RS1(1, K) = CBRT(3, /4, /3, 1416*RS(1, K-1)) + 3*DVS1(1)
000049          10, RS1(1, 1) = 0,
000050          10, RS1(1, K) = CBRT(3, /4, /3, 1416*RS(1, K-1)) + 3*DVS1(1)
          CR3(1, 1) = 3, 1416*RS(1, 1) + 3*DVS1(1)
          DO 11 K = 2, NDR4
          CR1(1, K) = DVS(1) * RHOS(1)
          CR2(1, K) = 3, 1416*RS(1, 1, 2*K-2) + 2*DIF1 / (RS1(1, 2*K-1) - RS1(1, 2*K))
000052          13) * RHOS(1)
000053          11, CR3(1, K) = 3, 1416*RS(1, 1, 2*K) + 2*DIF1 / (RS1(1, 2*K+1) - RS1(1, 2*K+1))
000054          1) * RHOS(1)
          CR1(1, NDR4) = CR1(1, 1)
          CR1(2, NDR4) = CR1(2, 1)

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RETURN
END

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000060

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SUBROUTINE PROSES8

```

000001      C
000002      C
000003      C
000004      DIMENSION AVLD(41)
000005      COMMON /BLOK1/ ABED(41), A(41), AVC(41), CGP(41), RHOG(41),
000006      1HGX(41), HXS(41), HXC(41), DIF(41), F(41), C(41), VS(2), DIS(2),
000007      DVIS(2), R, DS(41), RHOIS(2), UG(41), WM(2), UC(41), NDXM, PS(41), RHOIS(41),
000008      CS1(2,41), CS2(41), C1(21,41), C2(21,41), D1(21,41), D2(21,41), PC1(41),
000009      PC2(41), PC3(41), ASG(41), ASX(41), AGX(41), C1B(41), C2B(41), CIP(41), DP(41),
000010      S, FR(2,41), R0(2,41), R0(2,NDX1), NDX4, DX, DT, DK(41), DH(41), SK(41), P1(41), P2(41),
000011      B(21,41), WS(41), CR1(2,21), CR2(2,21), CR(2,21), C1(21,41), B(21,41),
000012      CP1(41), CP2(41), X(41), Y(41), VOLDF(41), TIME
000013      A, AXCL(41), RHOC(41), CPC(41), T268, AX(X(41), TX(X(41)), CRX(41), RHDX(41),
000014      9, NDG, PK(2,41), PC021, PW201, GMR(MW, TG), PT(41), CPS(41), HSC(41)
000015      COMMON /BLOK3/, W(21,41), TS(41)+TS(41), TX(41), CYCLE
000016      DOUBLE PRECISION W
000017      COMMON /BLOKA/, POUT(10), TIMET(10), NBCOUT, NPSET(3)
000018      COMMON /BLOK6/, NCYCLT
000019      COMMON /BLOK8/, DTO-784+41)+282(41)+7X2(41)+TC1(41), TC2(41)+,
000020      COMMON /BLOK10/, PRINT, DMX, NOTCON
000021      COMMON /BLOK11/, TOTCO2, TOTM20, SUMPTM, VTACHS, ITSG
000022      COMMON /BLOK12/, NTEMP
000023      COMMON /BLOK13/, WI, TI
000024      COMMON /BLOK14/, NCYCLE
000025      COMMON /BLOK15/, NDXMAC, BCQAC, VOLCAS, BCQAC
000026      COMMON /BLOK17/, NSTART
000027      DIMENSION AXS(41), AXGLA(41), AGS(41), HAXL(41), HGX(41), HGS(41), ACX(41),
000028      1HCX(41)
000029      EQUIVALENCE (ASX, AXB), (AGX, AXC), (ASG, AGS), (HXS, HSX), (HXC, HCX), (WSG,
000030      1, HGS), (ACX, ACV), (HXC, HCX)
000031      DOUBLE PRECISION C1P, C2P, CJB, DSP
000032      DOUBLE PRECISION C1, C2, D1, D2, PC1, PC2, PC3, P1, P2, P3, C3, Q, B,
000033      1, CP1, CP2, X, DT
000034      EQUIVALENCE (NDX, NDX1)
000035      C
000036      TIME=6.400, CYCLE, TIME, TIMEH, DI
000037      WRITE (6,400), CYCLE, TIME, TIMEH, DI
000038      WRITE (6,101)
000039      WRITE (6,102), N, PT(N), TS(N), IC(N), IX(N), NR1(NDX)
000040      IP(( NPSET(1) . GT. 0) . OR. (NPSET(2) . GT. 0)) GO TO 99
000041      WRITE (6,200)
000042      WRITE (6,201), N, X(N), FR(1,N), FR(2,N), N, NR1(NDX)
000043      99 WRITE (6,202)
000044      N1=NDXM+1
000045      NDRA=NDRA-1
000046      DO 20 N= 1, NDXM
000047      SUMMS=0.0
000048      SUMMS=SUMMS+0.5*(W(1,N)*W(NDR4,N))
000049      IF(NDR4 .EQ. 2) .AVLD(N1) .EQ. 2 .SUMMS=
000050      WRITE (6,200)
000051      IF(NDR4 .EQ. 2) GO TO 20
000052      DO 22 NR=2,NDR4
000053      SUMMS=SUMMS+W(NR,N)
000054      22 SUMMS=SUMMS+NDR4
000055      DO 30 N=N1,NDXM
000056      SUMMS=0.0
000057      SUMMS=SUMMS+0.5*(W(1,N)*W(NDR4,N))
000058      IF(NDR4 .EQ. 2) .AVLD(N) = SUMMS

```



```

000059 IF(NDR4.EQ.2) GO TO 30
000060 DO 33 NR=2, NDR3
000061      33 SUMMASUMMS$((NR,N))
000062      AVLD(N)=SUMMS/NDR3
000063      30 CONTINUE
000064      IF(NDXMAC .EQ. 0) GO TO 35
000065      SUM=0.
000066      DO 31 N= 1, NDIMAC
000067      31 SUM=SUM+AVLD(N)*AED(N)*DX*RHOBIN)
000068      AVMSLD = SUR/WTACHS
000069      35 CONTINUE
000070      IF((NDX1-NDM) .EQ. 0) GO TO 40
000071      SUM=0.
000072      DO 32 N= N1,NDX1
000073      32 SUM = SUM+AVLD(N)*AED(N)*DX*RHOBIN)
000074      AVSGLD=SUM/WTGC
000075      40 CONTINUE
000076      DO 10 N=1,NDX
000077      10 WRITE (A,203)(W(NR,N),NR=1,NDR4)
000078
000079      WRITE (A,205) AVMSLD, AVSGLD
000080      IF(TIME .LT. 1.E-20) AVMSL1=AVMSLD
000081      IF(TIME .LT. 1.E-20) AVSGL1=AVSGLD
000082      AVRHO2=WATCIS*(AVMSL1-AVMSLD)/TIME
000083      AVRHO2=WTSGC*(AVSGL1-AVSGLD)/TIME
000084      WRITE(6,204) AVRHO2,AVRH20
000085      RETURN
000086      C      100 FORMAT (1H4,16HDESORPTION CYCLE,13/
000087      1      3H,5MTIME,F9.9,1X2HHR,F12.2,1X,3HMIN,
000088      1      3H,15MTIME,INCREMENT,F7.3,1X2HHR),
000089      101 FORMAT (/2X,10AXIAL NODE,1D,14HTOTAL PRESS,MM 0X,14HGAS TEMP,DE
000090      101          1G F,5X,19HCOBENT TEMP.,DEG F,2X,18HCOOLANT TEMP.,DEG F,3X,19HUX CO
000091      2RE TEMP , DEC F )
000092      102 FORMAT (1L19,11X,B(F14.4,6X))
000093      103 FORMAT (/2X,0C02 DESORPTION RATE=F7.4,1X5HLB/HR,5X,20H2O DESORPTI
000094      103          1ON RATE=F7.4,1X5HLB/HR),
000095      200 FORMAT ((1W02X,10AXIAL NODE,13X,9MMOLE FRAC,7X,
000096      200          12X,13HC02 RATE,M/HRO,X,13H2O RATE,M/HB),
000097      201 FORMAT ((/19,11X,214X,F12.6,4X))
000098      202 FORMAT (//,31HLOADING AT INTERIOR OF SORBENT//4X,4HSORB/4X,4HNOD
000099
000100      1E,3X, 3HAVG, 9X,
000101      1, 1H1.9X,1H2.9X,2H10,
000102      21H8.9X,1H9.6X,2H10,
000103      28X,2M1/6H AXIAL/5H NODE),
000104      203 FORMAT ( 15,4X,12(F6.4,4X))
000105      204 FORMAT (//22HOTIME AVG CO2 DEBOPR RATE +
000106      1, F8.4, 6W LB/HR ,10X,
000107      227H TIME AVG H2O DEBOPR RATE ,
000108      3 F8.4, 7W LB/HR ,
000109      205 FORMAT (//,10W AVG CO2 LOADING IN M.S. BED , F8.4,1X,5HLB/LB,7X,
000110      13DH AVG H2O LOADING IN S.C. BED , F8.4, 6W LB/LB)
000111      END

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000001      SUBROUTINE HXCCORE(TX,TC,TS,TG,HXC,HXS,HXG,RHOX,CPX,TKX,DY,DT,NDX,A
000002          IVX,NDXM),
000003
000004      C
000005      DIMENSION TX(1),TC(1),TS(1),TG(1),HXC(1),HXS(1),HXG(1),RHOX(1),
000006          1CPX(1),TKX(1),IVX(1)
000007      DIMENSION C1(41),C2(41),C3(41),D1(41)
000008      COMMON /BLOK8/ DTO,TS1(1),TS2(41),TX1(41),TC1(41),TC2(41)
000009      DN=DT-DTO
000010      DO 10 N=1,NDX
000011      T1= AVX(N)*(HAC(N)+HXS(N)+HXG(N))+0.5
000012      C1(N)=TKX(N)/DX/DX
000013      C3(N)= -TKX(N+1)/DX/DX
000014      C2(N)= RHOX(N)*CPX(N)/DN*TX2(N)-C1(N).+ C3(N).+ T1
000015      10 D1(N)= RHOX(N)*CPX(N)/DN*TX2(N)+AVX(N)*(HXC(N)
000016          + TS1(N)*HXS(N)*HXG(N)+TG(N))- T1*TX2(N)
000017          C2(1)=C2(1)+C1(1)
000018          C1(1)=0.
000019          C2(NDX)=C2(NDX)+C3(NDX)
000020          CALL FDEQIM(C1,C2,C3,D1,TX,NDX)
000021          RETURN
000022      END

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      SUBROUTINE LAGIN2(ID,XNP,ND,X0,Y0,Y)
      C           REVISED FOR FORTRAN IV 8-8-65  S. WONG
      C           DIMENSION X(2), Y(2)

      000001          C
      000002          C
      000003          C
      000004          C

      000005          IL0$1
      000006          4 IF(X0>X(NP))10,16,4
      000007          4 IF(X0<X(NP))19,13,7
      000008          7 IL0=NP-1
      000009          10 IM1$1=0+1
      000010          WRITE (6,1) ID,X0
      000011          GO TO 46
      000012          13 IL0=NP
      000013          16 Y0=Y(IL0)
      000014          RETURN
      000015          19 DO 22 IL0=2,NP
      000016          1F(IF(X0>X(IL0))25,16,22
      000017          22 CONTINUE
      000018          25 IM1$1=0
      000019          IL0$1=IL0+1
      000020          1F((ND-2)*46,46,28
      000021          26 DO 43 I=2,ND
      000022          1F((IL0-1)*40,40,31
      000023          31 1F(IM1-NP)34,37,39
      000024          34 1F((2*X0-X(IL0-1))*X(IM1+1)) 37,37,40
      000025          37 IL0$1=0+1
      000026          CO 70 43
      000027          40 IM1$1=1
      000028          43 CONTINUE
      000029          46 Y0D=0
      000030          PNP=1.0
      000031          47 DO 49 IL0=1,IM1
      000032          49 PN=PN*(X0-X(I))
      000033          50 DO 52 JEIL0=1,IM1
      000034          51 P=PN/(X0-X(I))
      000035          52 DO 55 JEIL0=1,IM1
      000036          53 1F((J-1)*52,53,52
      000037          52 P=P/(NP-1)
      000038          55 CONTINUE
      000039          56 Y0=PN*Y(I)
      000040          58 CONTINUE
      000041          59 RETURN
      000042          1 FORMAT (97X,7HLAGIN2 ,1,1E12.5)
      000043          END

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000001      SUBROUTINE ISORB
000002      COMMON /BL0K1/ ABED(41), A(41), VCG(41), RHOG(41),
000003           1HXC(41), HXS(41), HXC(41), D1F(41), F(41), C(41), VGS(2), DVS(2), R
000004           2S1(2,41), RHOS(2), UC(21,41), WM(2), UC(41), NDXM(P3(41), RHOB(41),
000005           3CS1(41), CS2(41), C1(21,41), C2(21,41), D1(21,41), D2(41), PC1(41), PC2(4
000006           41), PC3(41), SG(41), ASK(41), ACK(41), C1P(1), C2P(1), C3P(41), D1P(41)
000007           5, ER(2,41), RS(2), NDX1, NDRA, DM, DZ, DK(41), DH(41), SK(44), P1(41), P2(41),
000008           6, P3(41), WS(41), CR1(2,41), CR2(2,21), C3(21,41), B(21,41),
000009           7Q(21,41), CR1(41), CR2(41), X(41), Y(41), Z(41), X(41), Y(41), Z(41), TIME,
000010           8, AXC(41), RHOC(41), CPC(41), T268, AVX(41), TXN(41), CPX(41), RHOX(41),
000011           9, ADC, BK(2,41), PC021, PW201, GMR, GMN, TGL, PA, PI(41), CPS(41), HAC(41)
000012      DOUBLE PRECISION C1, C2, D1, D2, PC1, PC2, PCS, P1, P2, P3, Q, B,
000013      C1+C2, X, Q,
000014      DOUBLE PRECISION C1P, C2P, C3P, D1P
000015      COMMON /BL0K3/ M(21,41), TC(41), TS(41), TC(41), TX(41), CYCLE
000016      DOUBLE PRECISION W
000017      COMMON /BL0K5/ DTO, TS4(41), TS2(41), TS1(41), TC1(41), TC2(41)
000018      DIMENSION S1(41), S2(41), S3(41), B1(41)
000019      DO 10 N=1, NDY
000020      T=(DT*DTO)/CP3(N)/RHOB(N)
000021      T1=0.5*T*(ASGN(N)*HSG(N)*ASK(N)*HXS(N))
000022      CB1(N)=C81(N)*(1.0+T1)
000023      CB2(N)=C82(N)*(1.0+T1),
000024      B1(N)=TS2(N)*C81(N)*P1(N)*C82(N)+(P1(N)*P2(N)*(W*NDR4,N)-W(N))/C81(N)*HXS(N)*HYS(N)
000025      1P3(N)=P1(N)*C82(N)*ASG(N)*HSG(N)*ASK(N)*HXS(N)*HYS(N)
000026      2
000027      IF(N,80,1) S1(N)=0.0
000028      1P(N,80,1) GO TO 11
000029      S1(N)=TOSK(N)/DX/DX*(ABED(N+1)+ABED(N))/(2.*ABD(N))
000030      11 S3(N)=TOSK(N)/DX/DX*(ABED(N+1)+ABED(N))/(2.*ABD(N))
000031      S2(N)=1.-S1(N)-S3(N)*A2
000032      10 CONTINUE
000033      CALL FDEQIN(S1,S2,S3,B1,T8,NDX1)
000034      RETURN
000035      END

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END_CUR UCC_1/A



PART II

MULTIPLE BED PROGRAM (MAIN4B)



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NOMENCLATURE

<u>FORTRAN</u>	<u>Algebraic*</u>	<u>Description</u>
A	$\left(\frac{f \cdot \rho_g \cdot u_g}{P \cdot M_g} \right)$	Quantity $\left(\frac{f \cdot \rho_g \cdot u_g}{P \cdot M_g} \right)$ appearing in Equation (2-35), Ref. (1) (1b-mole)/(hr)(sq ft) (mm Hg)
ADT		Temporary storage for DT, hr
ADT2		Temporary storage for DT, hr
ABED	A	Cross-sectional area of adsorbent bed, sq ft
AGS, ASG	a_{sg}	External surface area of sorbent, sq ft/(cu ft of bed)
AGX, AXG	a_{xg}	Primary heat transfer area between heat exchanger and gas stream, sq ft/cu ft of sorbent bed
ASX, AXS	a_{xs}	Primary heat transfer area between heat exchanger and sorbent, identical to a_{xg}
AVC	a_{vc}	Primary heat transfer area for coolant, sq ft/(cu ft of coolant volume)
AVLD		Average loading at each axial node, (1b-sorbate)/(1b- sorbent)
AVH2OP		Average poisoning rate of molecular sieves by H_2O , (1b- H_2O)/hr
AVMSLD		Average CO_2 -loading of all active molecular sieve sorbents, 1b- CO_2 /(1b-molecular sieves)
AVPH2O		Average outlet P_{H_2O} , mm Hg
AVRCO2		Average CO_2 adsorption or desorption rate, 1b- CO_2 /hr
AVRH2O		Average H_2O adsorption or desorption rate, 1b- H_2O /hr
AVSGLD		Average H_2O -loading of desiccant sorbents, 1b- H_2O / (1b-desiccant)
AVX	a_{vx}	Primary heat transfer area for heat exchanger, sq ft plate area/(cu ft of metal)

*Referring to equations in Part I of this report.



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<u>FORTRAN</u>	<u>Algebraic</u>	<u>Description</u>
B		Temporary variable used in simultaneous solution of a system of finite difference equations. See Equations (2-41) and (2-42), in Part I of this report.
C	C	Molal density of gas mixture, lb moles/(cu ft)
CPC	c_{pc}	Heat capacity of coolant, Btu/({}^{\circ}F)(lb)
CPG	c_{pg}	Heat capacity of gas mixture, Btu/({}^{\circ}F)(lb)
CPL		Specific heat of adsorbed sorbate, Btu/({}^{\circ}F)(lb)
CPP		Specific heat of dry sorbent, Btu/({}^{\circ}F)(lb)
CPS	c_{ps}	Sorbent specific heat, Btu/(lb)({}^{\circ}F)
CPX	c_{px}	Heat capacity of heat exchanger metal, Btu/{}^{\circ}F(lb)
CPI	{}	Coefficients in equation
CP2	{}	$PC3 \cdot (P_{ks,t} + \Delta t)^{-x_k P_t + \Delta t} = CPI + CP2 \cdot P_t + \Delta t$
CRI	{}	Coefficients in following equation which is merely another form of Equation (2-28), in Part I of this report.
CR2	{}	$CRI \cdot \frac{w_{k,M,(t + \Delta t)} - w_{k,M,t}}{(\Delta t)} = CR2 \cdot (w_{k,(M-1),(t + \Delta t)}$
CR3	{}	$-w_{k,M,(t + \Delta t)} + CR3 \cdot (w_{k,M,(t + \Delta t)}$
CSI	{}	$-w_{k,(M+1),(t + \Delta t)})$
CS2		$T_s(t + \Delta t) - T_s,t = DS + CSI \cdot P(t + \Delta t)$
		$- CS2 \cdot P_{ks,(t + \Delta t)}$
CYCLE		Cycle time per one adsorption or one desorption half-cycle, hr
C1	{}	Coefficients in equation
C2	{}	$C_1 \cdot w(t + \Delta t), (M-1) + C2 \cdot w(t + \Delta T), M$
C3	{}	$+ C3 \cdot w(t + \Delta t), (M+1) = DI$



<u>FORTRAN</u>	<u>Algebraic</u>	<u>Description</u>
C1P		Coefficients in equation
C2P		$C1P \cdot P(t + \Delta t), (N-1) + C2P \cdot P(t + \Delta t), N$
C3P		$+ C3P \cdot P(t + \Delta t), (N + 1) = DIP$
DH	ΔH	Heat of adsorption at each node Btu/(1b adsorbed)
DIF	D_k	Mass diffusivity of component k through the interior of sorbent, sq ft/hr
DP		Sorbent diameter, ft
DPC02C		Cabin CO_2 partial pressure increase in one time increment, mm Hg
DS		See CSI
DT	Δt	Time increment, hr
DTMAX		Maximum allowable time step size, usually 0.01 hr for isothermal analysis and 0.005 hr for nonisothermal analysis
DT0		Time increment of previous computation step, hr
DTT		Maximum allowable time increment calculated from each bed transient, hr
DVS		Size of interior sorbent volume elements, (cu ft)
DVSI		Size of sorbent volume elements at surface and center of spherical pellets, DVSI = 1/2 DVS, (cu ft)
DX		Axial node dimension, ft
DI		See CI
DIP		See C1P
D2		Coefficient in equation $W_{ks}(t + \Delta t) = Q + D2 \cdot P(t + \Delta t)$
F	F	Factor defined by Equation (2-17), a function of pressure
FR		Molar flow rates of CO_2 and H_2O , during desorption, FR (1,N) is CO_2 rate, FR (2,N) is H_2O rate, lb-mole/hr



<u>FORTRAN</u>	<u>Algebraic</u>	<u>Description</u>
G		Mass flux = $u_g \cdot \rho_g$, lb/(hr)(sq ft void area)
GK	K_g	Mass transfer coefficient between bulk stream and the surface of adsorbent. Surface kinetic rate can be incorporated in this coefficient, lb-moles/(hr)(sq ft)(mm Hg)
GMR	G_t	Total mass flow rate, lb/(hr)
GMRI		
GMR2		
GMR3		
GMR4		
GMW	M_g	Average molecular weight of process gas
GMW1		
GMW2		
GMW3		
GMW4		
HCX, HXC	h_{xc}	Heat transfer coefficient between heat exchanger primary plate and coolant, Btu/(sq ft)(°F)(hr)
HGS, HSG	h_{sg}	Heat transfer coefficient between sorbent and gas, based on a_{sg} , Btu/(sq ft)(°F)(hr)
HXS, HXS	h_{xs}	Effective heat transfer coefficient between heat exchanger primary plate and sorbent, Btu/(sq ft)(°F)(hr)
HTR		Same as HTRI if ISTOPC = 0. This variable is used in program
HTRI		Electric heater power read-in for each node, Btu/hr
HXG		Heat transfer coefficient between heat exchanger primary plate and gas stream, Btu/(sq ft)(°F)(hr)
IDB		Storage variable for all the integer variables characterizing desiccant bed configurations, such as NPSET, NDR4, etc
IDSORB		Index identifying sorbent used for each node; 1 = 5A, 2 = S.G. 3 = 13 X, 4 = 4A, 5 = 3A
IMAIN		Storage variable for the control integer variables for the system, such as NCYCLT, NPRINT, etc



<u>FORTRAN</u>	<u>Algebraic</u>	<u>Description</u>
IMB		Storage variable for all the integer variables characterizing molecular sieve bed configurations, such as NPSET, NDR4, etc
ISTOPC		Control index showing availability of coolant and heat, if $ISTOPC \neq 0$, $WC = 0$, $HTR = 0$, $SABC02 = 0$
KBED		Integer indicating whether a bed exists. $KBED(3) = 0$ means bed 3 does not exist
NCT1		Number of cycles to be run before assessment of water poisoning effects
NCT2		Number of cycles to be run after node adjustment for effects of water-poisoning
M_{sg}		Molal rate of mass transfer into bulk gas stream/unit bed volume, lb-moles per (cu ft of bed) (hr); see Equation (2-15), in Part I of this report.
M_s		Interior node corresponding to the surface of pellet
NBCOUT		Integer control variable, if $NBOUT = 2$, the outlet manifold pressure is specified as a function of time; $NBOUT = 1$, the manifold pressure is computed from vacuum duct resistance
NCYCLE		Number of complete adsorption-desorption cycles from beginning of run
NCYCLT		Total number of complete adsorption-desorption cycle calculations desired
NDR4		Integer denoting total number of radial sorbent pellet nodes (interior nodes)
NDTCON		If = 1, internal Δt calculations. If = 2, fixed Δt 's in program will be used
NDXM		Integer denoting total number of molecular sieve nodes
NDXMAC		Integer denoting number of active molecular sieve modes, i.e., $(NDXM-NDXMAX)$ represents the number of molecular sieve nodes which have been inactivated by water poisoning
NDXI		Integer denoting total number of axial nodes



<u>FORTRAN</u>	<u>Algebraic</u>	<u>Description</u>
NHALF		NHALF = 1, beds 1 and 2 are adsorbing, beds 3 and 4 are desorbing; NHALF = 2, beds 1 and 2 are desorbing, and beds 3 and 4 are adsorbing
N0G		Node to which coolant is added
NPR		Number of time steps elapsed since last printout
NPRINT		Integer control variable which determines the frequency of printout occurrence; e.g., if NPRINT = 5, printout occurs after every five time steps
NPSET		Integers which denote the nodes to which tabulated vacuum history is applicable
NSTART		Integer denoting the cycle from which on bed performance will be printed at frequency specified by NPRINT
NST1		NSTART for the NCT1 run
NST2		NSTART for the NCT2 run
NTEMP		Integer control variable; if NTEMP = 0, the energy equations will be ignored and bed temperatures set equal to TCIN; if NTEMP ≠ 0, heat balances will be performed
PA	P	Bed total pressure during adsorption, mm Hg
PAC		Cabin pressure, mm Hg
PA1	{	PA for bed 1, bed 3, bed 3 and bed 4, respectively
PA2		
PA3		
PA4		
PC02A		CO ₂ -accumulator pressure, psia
PC02C		CO ₂ partial pressure in cabin, mm Hg
PC02I		CO ₂ partial pressure at adsorption bed inlet, mm Hg
PC02I1	{	PC02I for bed 1, bed 2, bed 3 and bed 4, respectively
PC02I2		
PC02I3		
PC02I4		

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<u>FORTRAN</u>	<u>Algebraic</u>	<u>Description</u>
PCI		Coefficients in equation for desorption pressure
PC2	$\frac{P(t+\Delta t), N - P_t, N}{(\Delta t)}$	
PC3	$= PCI \cdot \frac{P(t+\Delta t), N-1)^{-2} P(t+\Delta t), N + P(t+\Delta t), (N-1)}{(\Delta x)^2}$ $+ PC2 \cdot \frac{P(t+\Delta t), (N+1) - P(t+\Delta t), (N-1)}{2(\Delta x)}$ $+ PC3 \cdot [P_{ks}(t+\Delta t) - X_k P(t+\Delta t)]$	
PH20C		H_2O partial pressure in the cabin, mm Hg
PH20I		Inlet H_2O partial pressure, mm Hg
PH20I1		PH20I for bed 1, 2, 3 and 4, respectively
PH20I2		
PH20I3		
PH20I4		
PK(K,N)	P_k	$P \cdot X_k$; partial pressure of component k in bulk gas stream, mm Hg
PK1		PK for bed 1, 2, 3 and 4, respectively
PK2		
PK3		
PK4		
PN2		N_2 partial pressure for overboard loss computation
PN21		PN2 for bed 1, 2, 3 and 4, respectively
PN22		
PN23		
PN24		
P0UT		10 tabulated desorption outlet pressures at TIMET, mm Hg
P02		O_2 partial pressure for overboard loss calculations
P021		P_02 for bed 1, 2, 3, and 4, respectively
P022		
P023		
P024		
PS		Variable for a temporary storage of PT



<u>FORTRAN</u>	<u>Algebraic</u>	<u>Description</u>
PT	P	Total pressure in bulk gas stream, mm Hg
PT1 PT2 PT3 PT4	}	PT for bed 1, 2, 3 and 4, respectively
PUMP		Pressure ratios at which vacuum pump displacements VPUMP are tabulated
P1 P2 P3	}	Coefficients in equation $p_{ks}(t+\Delta t) = P1 + P2 \cdot (w_{k,s}(t+\Delta t) - w_{k,s,t}) + P3 \cdot P$
Q		Temporary variable like B. See Equations (2-43) and (2-44), Ref (1)
RB1M		Variable equivalent to TG1, PH20I1, etc
RB2M		Variable equivalent to TG2, PH20I2, etc
RB3M		Variable equivalent to TG3, PH20I3, etc
RB4M		Variable equivalent to TG4, PH20I4, etc
RC02C		Rate of CO ₂ generation in cabin, 1b CO ₂ per hr
RDB		Storage variable for real variables characterizing desiccant bed configuration
RDBA		Storage variable for real variables characterizing desiccant bed adsorption half cycle transfer processes
RDBD		Similar to RDBA for desorption half-cycles
RGAS	R	Gas constant, 554 (mm Hg) (cu ft)/(1b-mole)(°R)
RH0C	ρ_c	Coolant density, 1b/(cu ft)
RH0G	ρ_g	Gas density, 1b/(cu ft)
RH0S	ρ_s	Sorbent density, 1b/(cu ft particle)
RH0SB	ρ_{sb}	Sorbent bulk density, 1b/(cu ft bed volume)
RH0X	ρ_x	HX core metal density, 1b/(cu ft)

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<u>FORTRAN</u>	<u>Algebraic</u>	<u>Description</u>
RMAIN		Real variable equivalent to WM, CYCLE, etc., which are common to all beds
RMB		Storage variable for real variables characterizing molecular sieve bed configuration, such as ABED, AVC, etc.
RMBA		Storage variable for real variables characterizing molecular sieve bed transfer processes during adsorption half cycles, such as HXG, HXS, etc.
RMBD		Similar to RMBA for desorption half cycles
RS r_s		Average particle radius found from ρ_{sb} and a_{sg} , ft
RSI		Radius of spherical surface separating two interior sorbent volume elements, ft
SABCØS		A permanent storage for SABCØ2
SABCØ2		Rate of CO ₂ intake by a Sabatier reactor or equivalent, lb/hr
SK k_s		Effective thermal conductivity of sorbent bed, Btu/(hr) (sq ft) (⁰ F/ft)
SUMPTM		Quantity $\sum_t P_{H_2O}$, outlet $\cdot (\Delta t), (mm)(hr)$ t = zero
TC T_c		Coolant temperature, ⁰ F
TCØ2A		CO ₂ -accumulator temperature, ⁰ F
TCIN		Identical with T268, inlet coolant temperature, ⁰ F
TC01 TC02 TC03 TC04	{	Initial TC for bed 1, 2, 3 and 4, respectively
TC1		Coolant temperature at time, t - Δt
TC11 TC12 TC13 TC14	{	TC1 for bed 1, 2, 3, and 4, respectively

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<u>FORTRAN</u>	<u>Algebraic</u>	<u>Description</u>
TC2		Coolant temperature at time, $t - 2\Delta t$
TC21 TC22 TC23 TC24	}	TC2 for bed 1, 2, 3 and 4, respectively
TG	T_g	Gas temperature, $^{\circ}\text{F}$
TGC		Cabin temperature, $^{\circ}\text{F}$
TGHX		Maximum allowable temperature at molecular sieve bed inlet, above which an intercooler will be used to lower it to TGHX, $^{\circ}\text{F}$
TGI	T_{gi}	Inlet gas temperature for adsorption cycle, $^{\circ}\text{F}$
TGI1 TGI2 TGI3 TGI4	}	TGI for bed 1, 2, 3, and 4, respectively
TG1 TG2 TG3 TG4	}	TG for bed 1, 2, 3, and 4, respectively
TI		Maximum temperature change allowable per time increment in selecting Δt , $^{\circ}\text{F}$
TIME	t	Time from beginning of each adsorption or desorption period, hr
TIMEDS		Maximum desorption time beyond which ISTOPC will be set equal to 1, hr.
TIMEM		Time above in minutes
TIMET		10 times at which POUT are tabulated, hr
TKX	k_x	Thermal conductivity of heat exchanger core metal, Btu/(hr) (sq ft) ($^{\circ}\text{F}/\text{ft}$)
TMAX		Maximum allowable sorbent temperature, above which heater will be shut off, $^{\circ}\text{F}$
TOTCO2		Total amount of CO_2 adsorbed since beginning of adsorption period, lb



<u>FORTRAN</u>	<u>Algebraic</u>	<u>Description</u>
TOTH _T		Total heat added/removed by coolant, Btu
TOTH ₂₀		Total amount of H ₂ O adsorbed since beginning of adsorption period, lb
TOTKWH		Total KWH of electric power used by desorbing beds, KWH
TS T _s		Sorbent temperature, °F
TS01 TS02 TS03 TS04	}	Initial sorbent temperatures for bed 1, 2, 3, and 4, respectively
TS1		Sorbent temperature at time t - (Δt), °F
TS11 TS12 TS13 TS14	}	TS1 for bed 1, 2, 3, and 4, respectively
TS2		Sorbent temperature at time t-2 (Δt), °F
TS21 TS22 TS23 TS24	}	TS2 for bed 1, 2, 3, and 4, respectively
TX T _x		Heat exchanger core metal temperature, °F
TX01 TX02 TX03 TX04	}	Initial TX for bed 1, 2, 3, and 4, respectively
TX1		Heat exchanger core metal temperature at time t - (Δt), °F
TX11 TX12 TX13 TX14	}	TX1 for bed 1, 2, 3, and 4, respectively
TX2		Heat exchanger core metal temperature at time t-2 (Δt), °F
TX21 TX22 TX23 TX24	}	TX2 for bed 1, 2, 3, and 4, respectively



<u>FORTRAN</u>	<u>Algebraic</u>	<u>Description</u>
T268	T_{268}	Inlet coolant temperature, °F
UC	u_c	Coolant velocity, ft/hr
UG	u_g	Interstitial gas velocity, i.e., true gas velocity, ft/hr
VC02A		CO_2 -accumulator volume, cu ft
VMS		Total bulk volume of molecular sieve sorbents, cu ft
VØIDF	f	Void fraction of bed
VØLCAB		Cabin volume for atmosphere, cu ft; use VØLCAB = 10^{20} , for constant PC02C
VPUMP		Vacuum pump displacements tabulated at pressure ratios PUMP, cfm
VS		Volume of a single sorbent pellet, cu ft
VSG		Total bulk volume of desiccants, cu ft
W	w_k	Local loading of component k in sorbent, lb sorbate k/lb sorbent
WC		Coolant flow rate actually used in program, lb/hr
WCC		Coolant flow rate inputted, lb/hr
	$w_d(P)$	A function of pressure which represents the capacity of vacuum duct at duct inlet pressure of P mm, lb/hr
WI		Maximum loading change allowable per time increment in selecting Δt , lb/lb
WM	M_k	Molecular weight of component K. K = 1 and 2
WS		Temporary storage variable for W
WTACMS		Total weight of active molecular sieve sorbents, lb
WTMS		Total weight of molecular sieve sorbents, lb
WTSG		Total weight of desiccants, lb
W1 W2 W3 W4	}	W for bed 1, 2, 3 and 4, respectively



<u>FORTRAN</u>	<u>Algebraic</u>	<u>Description</u>
X	x_k	Mole fraction of component k in gas stream $k = 1$ refers to CO_2 in molecular sieve bed gas stream, and $K = 2$ refers to H_2O in desiccant bed gas stream
	x	Distance from molecular sieve bed end, ft
	Y	Any of bed properties, T_s , T_x , w_k , T_c , T_g

Subscripts

b	Bulk
c	Coolant
g	Gas stream
i	Inlet
k	Component k
M	Radial location index for sorbent interior nodes
N	Axial location index
s	Surface of sorbent
s	Sorbent
t	At time t
v	Volume
x	Heat exchanger

Superscripts

* Equilibrium quantity



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SECTION 6

GENERAL DESCRIPTION

INTRODUCTION

The AiResearch composite sorbent bed program S9960 (Part I of this report) was developed for analyzing vacuum-dump sorbent bed systems such as the RCRS (Regenerative Carbon Dioxide Removal System) for the Apollo Applications Program and the Airlock Program. More complicated systems are required for longer mission applications in which H_2O , CO_2 , or both must be saved. To accommodate more complex systems, program S9960 has been modified and expanded. The new program is identified as MAIN4B and will now accommodate 4-bed/ H_2O -save- CO_2 -dump and 4-bed/ H_2O -save- CO_2 -dump configurations as well as the original 2-bed/vacuum-dump configuration. A typical 4-bed thermal-swing system that uses coolant is shown in Figure 6-1.

Computational schemes of program MAIN4B are basically the same as those of program S9960, although modifications have been made and a number of new features added. These changes are described in Section 7, Technical Description.

The most significant new feature of program MAIN4B is prediction of the effects of coadsorption of water, CO_2 , oxygen, and nitrogen on the system beds. The gradual buildup of water on the CO_2 removal bed has a pronounced effect of lowering the adsorption efficiency of that bed. Methods have been incorporated into MAIN4B to quantitatively predict this coadsorption effect. Also important is that coadsorption of atmospheric gases, oxygen and nitrogen, leads to loss of the gases overboard from a vehicle when vacuum-dump systems are employed. The rate of loss of these gases is estimated as a function of process conditions.

PROGRAM INPUT

The input to MAIN4B is by means of eleven namelists. The lists include initial conditions, bed sizes, mass and heat transfer coefficients, etc. However, equilibrium data of various sorbate-sorbent pairs are all contained in subroutines EQPWT and FC0AD in the form of data statements. These may have to be changed if better data become available.

PROGRAM OUTPUT

Printed pages are the only output from the program. The output provides the following:

- (a) Bed size
- (b) Estimated overboard gas losses



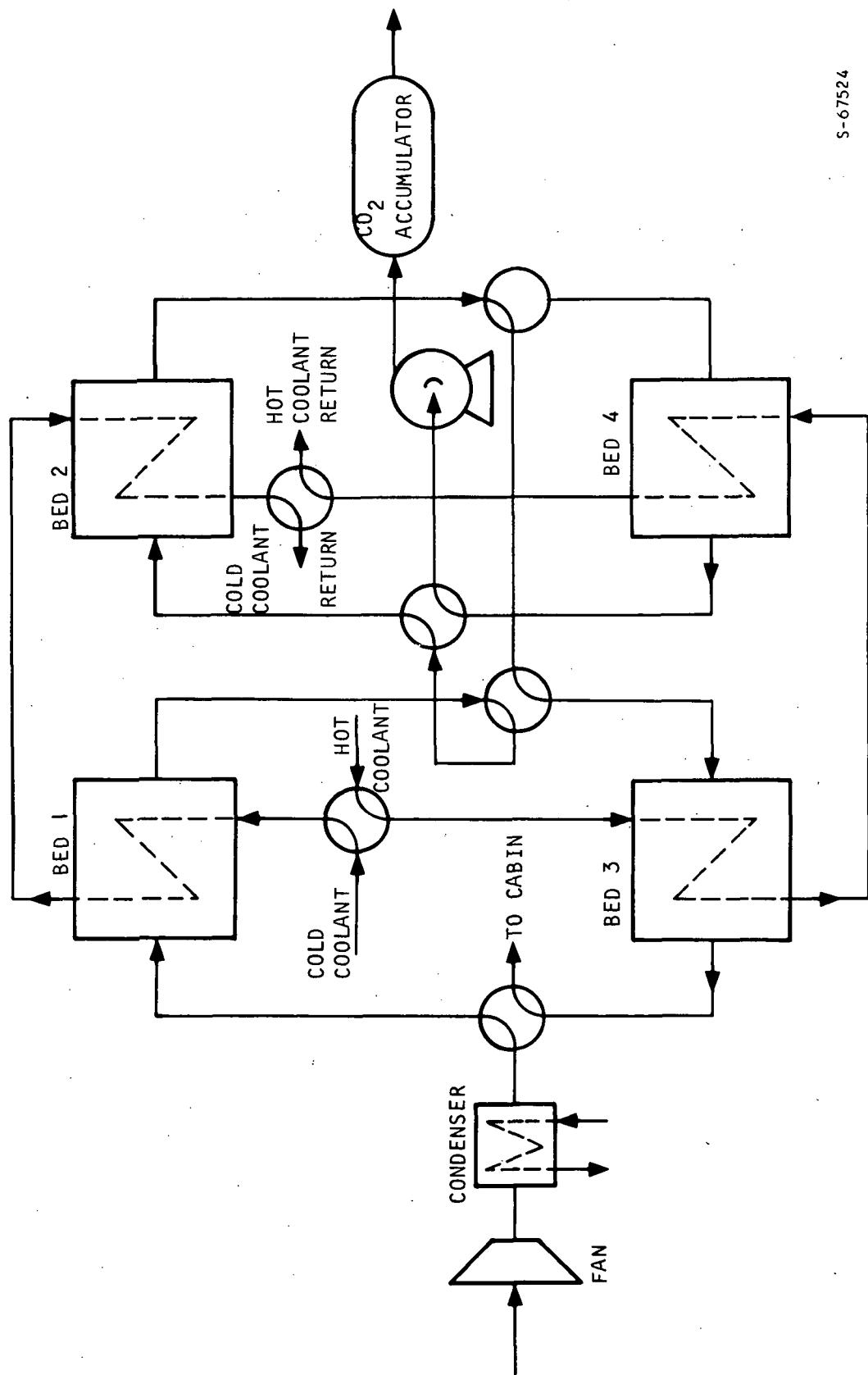


Figure 6-1. Typical 4-Bed Thermal Swing System



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- (c) Temperatures
- (d) Sorbate loadings
- (e) Average sorbate loadings
- (f) Average adsorption/desorption rates
- (g) Heat provided by electric heater and coolant
- (h) Sorbate partial pressures
- (i) Desorption pressures
- (j) CO₂-accumulator pressure and volume

The bed sizes and overboard gas losses are printed again after bed sizes are adjusted to account for water poisoning effects.

PROGRAM OPTIONS

Three categories of program options are listed below.

System Options

- (a) 2-bed-vacuum-dump
- (b) 4-bed-H₂O-save-CO₂-dump
- (c) 4-bed-H₂O-CO₂-save

Water-Poisoning Effects

- (a) Degree of poisoning known
- (b) Degree of poisoning to be found by the program and bed sizes adjusted accordingly

Individual Sorbent Bed Options

- (a) Isothermal operation with the bed temperature specified
- (b) Adiabatic operation
- (c) Thermal swing operation with hot and cold coolant
- (d) Thermal swing operation with an electric heater
- (e) Different sorbent and bed properties for different axial nodes
- (f) Desorption pressure specified as a function of time for up to three axial locations



- (g) Desorption bed outlet pressure computed from vacuum duct and pump characteristics
- (h) Desorption bed outlet pressure computed from input pump characteristics and CO₂ accumulator pressure.
- (i) Use of a constant pressure type CO₂-accumulator
- (j) Use of a constant volume type CO₂-accumulator



SECTION 7

TECHNICAL DESCRIPTION

INTRODUCTION

The technical description of program MAIN4B includes only the new features which have been added to program S9960. Basic heat and mass transfer models used in the program were described in Part I of this report.

VACUUM DUCT CHARACTERIZATION

In program S9960, an empirical correlation between duct inlet pressure and throughput was used to predict bed outlet pressures during desorption. As the correlation was based on conditions which are not universally valid, a generally applicable method was developed for the new program, MAIN4B.

In the modified analysis, the boundary condition is treated in a more general and rigorous fashion. Volumetric flow at the outlet face of the bed is calculated from pump displacement and flow conductance of the vacuum duct by

$$S = \frac{S_p C}{S_p + C} \quad (7-1)$$

where S = volumetric flow rate at the bed outlet, liters/sec

S_p = pump displacement, a function of pump inlet pressure, liters/sec

C = duct conductance, liters/sec

The duct conductance is calculated by

$$C = 3.269 \times 10^{-2} \frac{P_{av} D^4}{L\eta} + 3.81 \left(\frac{D^3}{L} \right) \left(\frac{T}{M} \right)^{\frac{1}{2}} \frac{1 + 0.147 \left(\frac{M}{T} \right)^{\frac{1}{2}} P_{av} \left(\frac{D}{\eta} \right)}{1 + 0.181 \left(\frac{M}{T} \right)^{\frac{1}{2}} P_{av} \left(\frac{D}{\eta} \right)} \quad (7-2)$$

where P_{av} = average duct pressure, torrs

D = duct diameter, cm

L = duct length, cm

M = molecular weight

T = temperature, °K

η = viscosity, poise



The characteristics of the vacuum pump used in Airlock Regenerative Carbon Dioxide Removal System qualification tests are used in the DESORB subroutine. The data statements characterizing the pump can be easily changed for different pumps. In the case of space vacuum, the pump displacements can be set to arbitrarily large quantities to simulate the almost unlimited capacity of space. The duct diameter and length set in DESORB can also be changed for different configurations.

PUMPING INTO A CO₂-ACCUMULATOR

For a CO₂-save system, MAIN4B allows the user to specify pump characteristics in the form of displacements vs pressure ratios - VPUMP vs PUMP. The line pressure drop is neglected in this case and the boundary condition used for the bed outlet is

$$-\frac{fA}{F} \left(\frac{\partial p}{\partial x} \right) = V_p \quad (7-3)$$

where f = void fraction

A = cross-sectional area of bed

F = bed resistance defined in Part I of this report

p = pressure, mm Hg

X = axial distance, ft

V_p = pump displacement, (cu ft)/hr

ENERGY EQUATION FOR HEAT EXCHANGER CORE METAL WITH EMBEDDED ELECTRIC HEATER

Program MAIN4B allows for the use of electric heaters embedded in heat exchanger metal. The new energy equation incorporating the heater is

$$\left(c_{px} \cdot \rho_x \right) \frac{\partial T_x}{\partial t} = \frac{\partial}{\partial x} \left(k_x \frac{\partial T_x}{\partial x} \right) + a_{vx} \cdot \left[h_{xs} \left(T_s - T_x \right) + h_{xg} \left(T_g - T_x \right) + h_{xc} \left(T_c - T_x \right) \right] + \dot{Q}_v \quad (7-4)$$

where the heat source \dot{Q}_v is the heater capacity in Btu/(cu ft of HX metal)

WATER POISONING OF SORBENT

Effects of the poisoning of molecular sieve sorbents 5A and 13X by water are shown in Figures 7-1 and 7-2. These data are set up in subroutine FC0AD, in the form of H₂O loading vs CO₂ capacity as a fraction of dry sorbent capacity. Expansion of the built-in data to include coadsorption data for other sorbents can be easily done whenever such data become available.



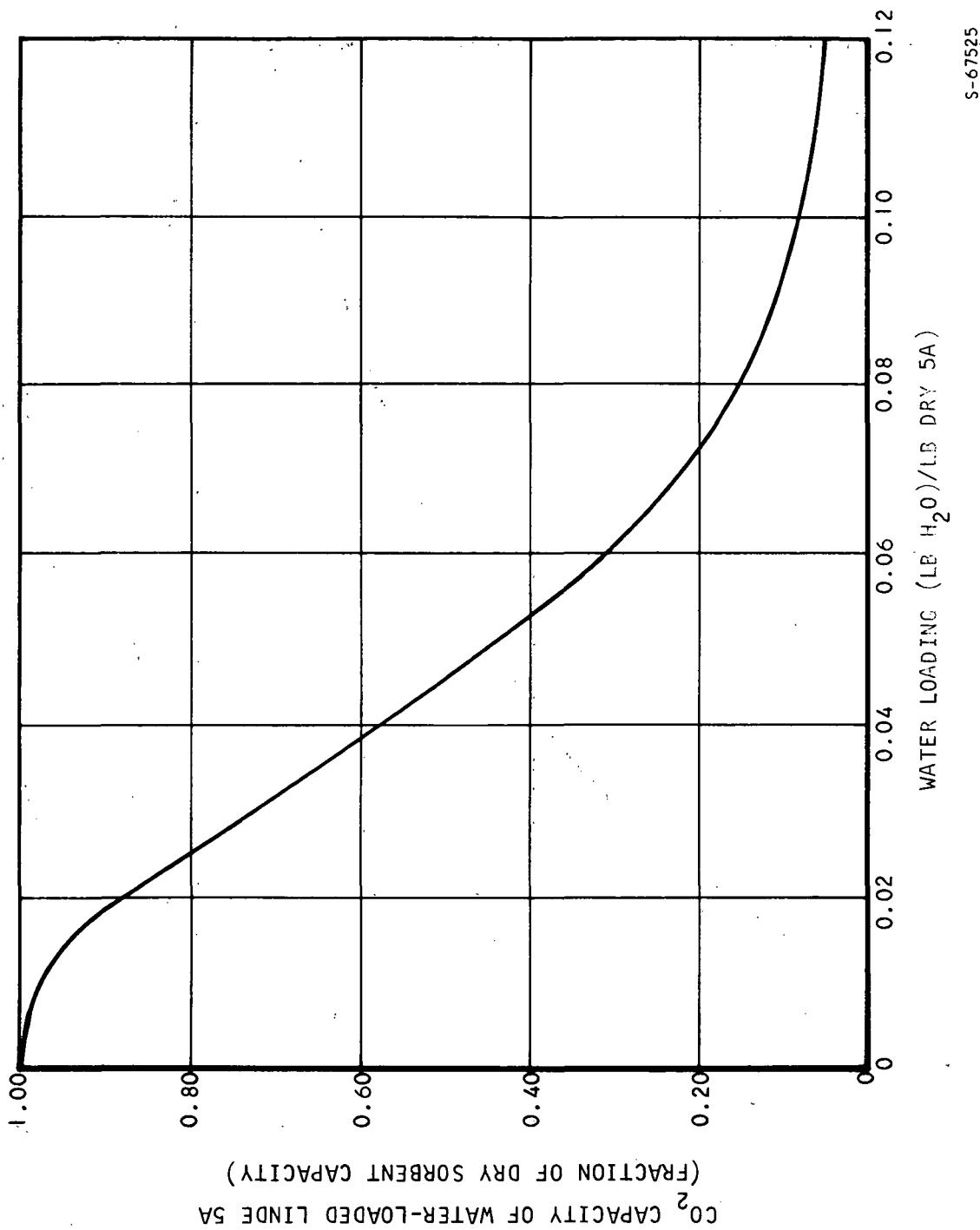


Figure 7-1. Effect of Water Poisoning on
Linde 5A Capacity for CO₂



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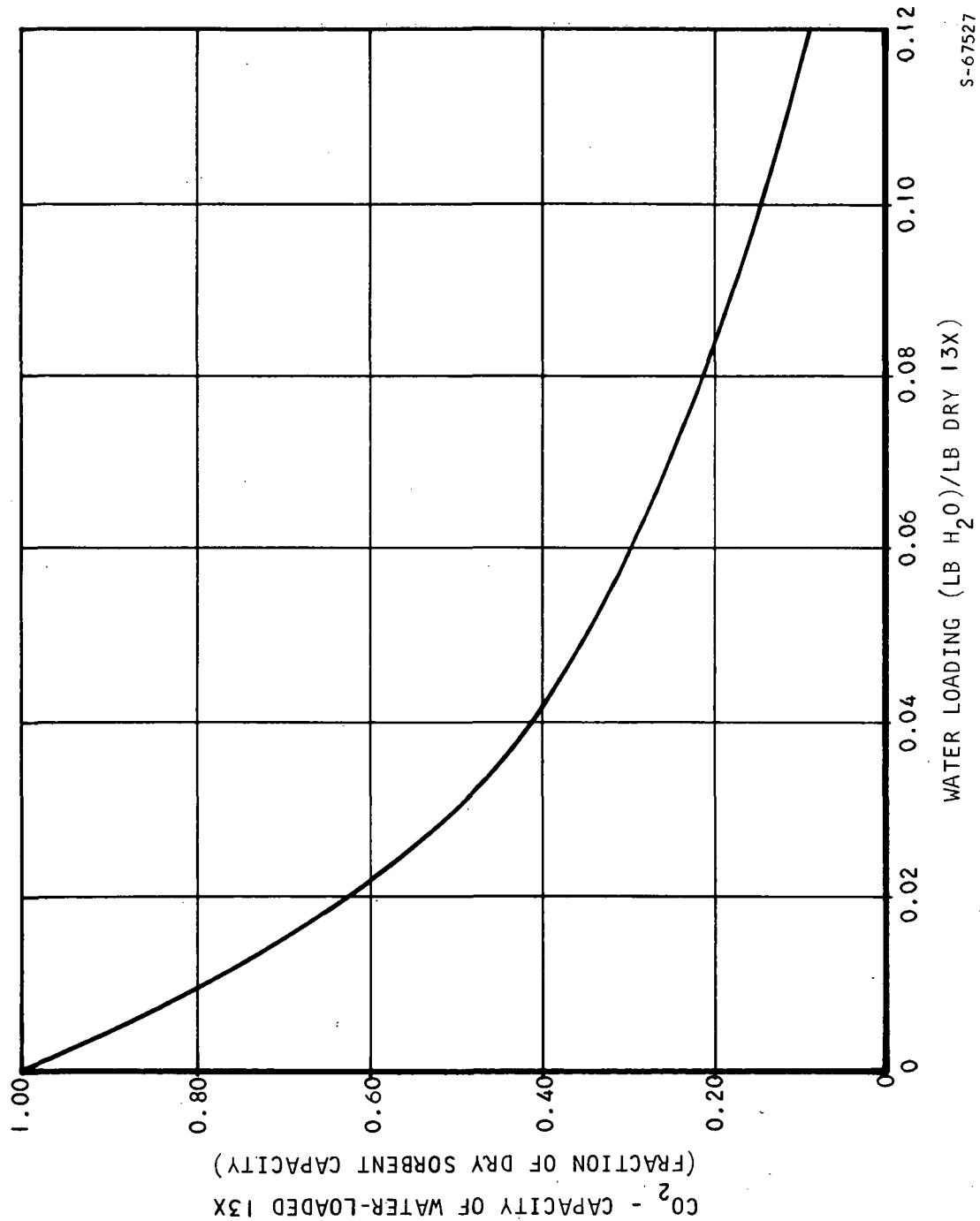


Figure 7-2. Effect of Water Poisoning on
Linde 13X Capacity for CO₂



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OVERBOARD GAS LOSSES

Overboard gas losses are estimated by assuming that, for molecular sieve sorbents 5A and 13X, the percentage reduction in capacity due to water poisoning is the same for CO_2 , N_2 and O_2 .

MAIN PROGRAM MAIN4B

The main program MAIN4B was written for a typical $\text{CO}_2\text{-H}_2\text{O}$ -sorbent thermal swing 4-bed system, depicted in Figure 6-1. A logic diagram of the program is shown in Figure 7-3. The program first determines the amount of water accumulated in each bed during the first NCT1 cycles.

In the input data, NDXM and NDXMAC for each bed are selected so that the CO_2 sorbent nodes which may potentially be poisoned in NCT1 cycles are assigned as desiccant nodes. This results in a desiccant section greater, and a CO_2 -sorbent section smaller, than the actual sizes. The program is run for NCT1 cycles to let water accumulate in the back end of the desiccant section, which in actuality is the front end of the CO_2 -section. This method predicts slightly less than actual performance of the CO_2 -removal bed. However, in the first half of the run, i.e., for the first NCT1 cycles, only the desiccant bed performance is of primary interest, and an approximate simulation of the CO_2 bed should suffice in estimating bed poisoning.

At the end of the NCT1 cycles, during which period the accumulation of water in the front part of the CO_2 -bed has been established, the effective dry sorbent quantity for CO_2 adsorption is found for each desiccant node, using the data presented in Figures 7-1 and 7-2. The total of all these equivalent dry sorbent weights is added to the CO_2 -sorbent section by resetting NDXM and NDXMAC. In case a non-integral number of desiccant nodes results, desiccant densities are adjusted to keep the total weight unchanged. Mass diffusivity, mass transfer coefficient and heat of adsorption (DIF, GK, DH) for the reassigned nodes are set to those of node No. 1.

After the resetting of the beds, the program is run for additional NCT2 cycles to establish the CO_2 removal performance of the bed with the degree of poisoning established in the first stage of the run. NCT2 is selected just large enough to give a stabilized solution.

In Figure 7-3, the 4-bed performance prediction is performed by the operations enclosed in the broken-line rectangle, which are shown in the right hand portion of the figure.



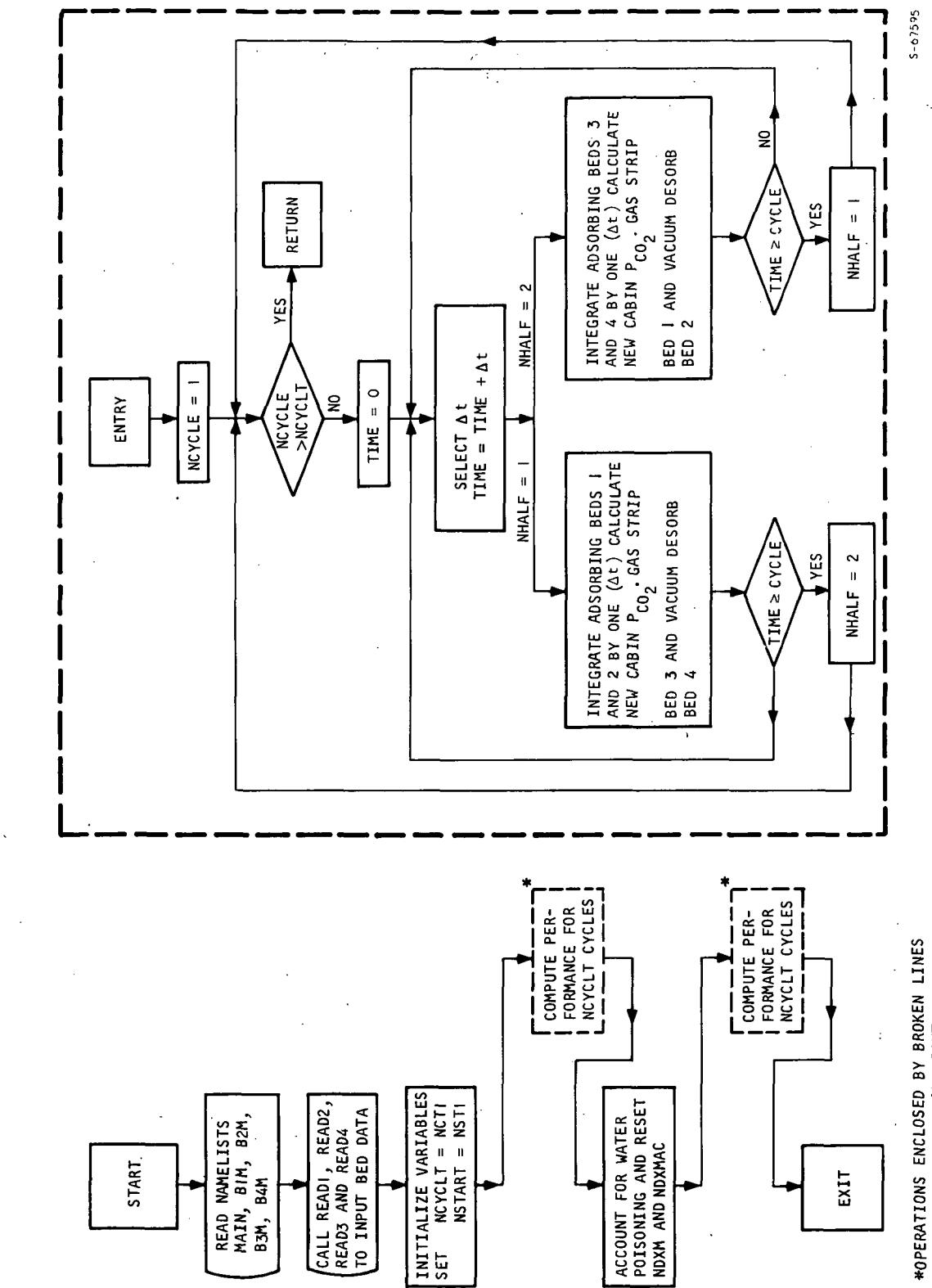


Figure 7-3. MAIN(B) Program Logic

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SECTION 8

USAGE

PROGRAM INPUT

All data required for program execution are inputted via eleven namelists. The following paragraphs describe the function of each namelist and define parameters/variables in the namelists.

Function of Various Namelists

Parameters defining the system and execution mode, common to all the beds, are contained in the namelist 'MAIN'. These include, among others, molecular weights of sorbates, half-cycle time, CO_2 -accumulator volume, and number of cycles to be run before the effect of water-poisoning will be evaluated.

Initial conditions, gas flow rates, P_{N_2} and P_{O_2} for each bed are included in namelists 'BIM', 'B2M', 'B3M', and 'B4M', respectively.

Desiccant bed characteristics, such as bed and sorbent sizes, various areas, sorbent-type used for each node, desorption mode to be used, etc., make up the namelist 'DB'.

Data characterizing desiccant bed mass and heat transfer processes, are included in 'DBA' for the adsorption half-cycle and 'DBD' for the desorption half-cycle.

Similarly, corresponding data for the molecular sieve beds are contained in the namelists 'MB', 'MBA' and 'MBD'.

Input Variable Lists and Definition1. Namelist MAIN

<u>Fortran Symbol</u>	<u>Definition</u>
WM(2)	Adsorbate molecular weight; eg., WM(1) = (CO_2) , WM(2) = 18(H_2O)
CYCLE	Cycle time per one adsorption or one desorption, period, hr
DTMAX	Maximum allowable time step size, usually 0.01 hr for isothermal analysis and 0.005 hr for nonisothermal analysis
WI	Maximum loading change allowable per time increment in selecting Δt , lb/lb



TI	Maximum temperature change allowable per time increment in selecting Δt , $^{\circ}$ F
PC \emptyset 2C	Initial CO_2 partial pressure in cabin, mm Hg
V \emptyset L \emptyset CAB	Cabin volume for atmosphere, cu ft; use $V\emptyset L\emptyset CAB = 10^{20}$, for constant PC \emptyset 2C
RC \emptyset 2C	Rate of CO_2 generation in cabin, lb CO_2 per hr
NPRINT	Integer control variable which determines frequency of printout occurrence; e.g., if NPRINT = 2, printout occurs after every two time steps
NDTC \emptyset N	If NDTC \emptyset N = 1, Δt will be selected such that $\Delta T = TI$, $\Delta W = WI$ for time step; if NDTC \emptyset N = 2, ΔT 's as set in program will be used
NTEMP	Integer control variable; if NTEMP = 0, isothermal analysis; the energy equations are ignored, and the bed temperature is set equal to TCIN. If NTEMP \neq 0, nonisothermal analysis
TGC	Cabin temperature, $^{\circ}$ F
PAC	Cabin pressure, mm Hg
PH \emptyset 2C	Cabin P_{H_2O} , mm Hg
TGHX	Maximum temperature allowable for CO_2 -beds inlet gas, if the temperature is exceeded, a gas cooler will be employed to lower the temperature to TGHX.
PC \emptyset 2A	CO_2 accumulator pressure, for a fixed volume type, psia
VC \emptyset 2A	CO_2 accumulator volume for a fixed pressure type, cu ft
SABC \emptyset 2	CO_2 flow-rate to Sabatier reactor, lb CO_2 /hr.
TC \emptyset 2A	CO_2 accumulator temperature, $^{\circ}$ F



KBED(4)	Index indicating whether a bed exists. E.g., if only bed 2 exists, KBED = 0, 1, 0, 0
TIMEDS	If TIMEDS<CYCLE, heat is available only during TIMEDS of the desorption half-cycle, beyond TIMEDS hot coolant, electric heater will be shut off.
NCT1	Total number of complete adsorption-desorp- tion cycle calculations desired before effects of bed-poisoning will be assessed and bed sized adjusted accordingly to pre- dict bed performance.
NST1	Cycle at which print-out will be started for the aforementioned run.
NCT2	Total number of complete adsorption- desorption cycle calculations desired after bed adjustments for poisoning.
NST2	Cycle at which print-out will be started for the run with adjustments for poisoning.

2. Namelist BIM

<u>Fortran Symbol</u>	<u>Definition</u>
PAI	Bed No. 1 total pressure, mm Hg
TSOI(20)	Bed No. 1 initial sorbent temperature, °F
TCOI(20)	Bed No. 1 initial coolant temperature, °F
TXOI(20)	Bed No. 1 initial HX metal temperature, °F
WI (4,20)	Bed No. 1 initial sorbate loading, 1st subscript denoting sorbent interior radial nodes; 2nd subscript denoting axial nodes; lb sorbate/lb dry sorbent.
GMR1	Bed No. 1 process gas flow rate, lb/hr
GMWI	Bed No. 1 process gas molecular weight
PN21	Bed No. 1 N ₂ partial pressure, mm Hg
P021	Bed No. 1 O ₂ partial pressure, mm Hg



3. Namelist B2M

<u>Fortran Symbol</u>	<u>Definition</u>
PA2	Bed No. 2 total pressure, mm Hg
TS02(20)	Bed No. 2 initial sorbent temperature, °F
TC02(20)	Bed No. 2 initial coolant temperature, °F
TX02(20)	Bed No. 2 initial HX metal temperature, °F
W2(4,20)	Bed No. 2 initial sorbate loading, 1st subscript denoting sorbent interior radial nodes; 2nd subscript denoting axial nodes; 1b sorbate/lb dry sorbent.
GMR2	Bed No. 2 process gas flow rate, lb/hr
GMW2	Bed No. 2 process gas molecular weight
PN22	Bed No. 2 N ₂ partial pressure, mm Hg
PØ22	Bed No. 2 O ₂ partial pressure, mm Hg

4. Namelist B3M

<u>Fortran Symbol</u>	<u>Definition</u>
PA3	Bed No. 3 total pressure, mm Hg
TS03	Bed No. 3 initial sorbent temperature, °F
TC03	Bed No. 3 initial coolant temperature, °F
TX03	Bed No. 3 initial HX metal temperature, °F
W3	Bed No. 3 initial sorbate loading, 1st subscript denoting sorbent interior radial nodes, 2nd subscript denoting axial nodes, 1b sorbate/lb dry sorbent.
GMR3	Bed No. 3 process gas flow rate, lb/hr.
GMW3	Bed No. 3 process gas molecular weight.
PN23	Bed No. 3 N ₂ partial pressure, mm Hg.
PØ23	Bed No. 3 O ₂ partial pressure, mm Hg.



5. Namelist B4M

<u>Fortran Symbol</u>	<u>Definition</u>
PA4	Bed No. 4 adsorption cycle total pressure, mm Hg
TS04	Bed No. 4 initial sorbent temperature, °F
TC04	Bed No. 4 initial coolant temperature, °F
TX04	Bed No. 4 initial HX metal temperature, °F
W4	Bed No. 4 initial sorbate loading, 1st subscript denoting sorbent interior radial nodes, 2nd subscript denoting axial nodes; lb sorbate/lb dry sorbent.
GMR4	Bed No. 4 process gas flow rate, lb/hr.
GMW4	Bed No. 4 process gas molecular weight.
PN24	Bed No. 4 adsorption cycle N ₂ partial pressure, mm Hg.
P024	Bed No. 4 adsorption cycle O ₂ partial pressure, mm Hg.

6. Namelist DB

<u>Fortran Symbol</u>	<u>Definition</u>
ABED (20)	Sorbent bed cross-section area normal to flow of process gas, sq ft
AVC (20)	Primary heat exchanger plate area per unit volume of coolant held up in HX, sq ft/(cu ft)
ASX (20)	Heat exchanger primary area per unit volume sorbent bed, sq ft/(cu ft)
AGX (20)	Identical to ASX
AVX (20)	Primary heat exchanger plate area per unit volume of heat exchanger core metal, sq ft/(cu ft)
RH0G (20)	Gas density, lb/(cu ft)



RH ₀ SB (20)	Sorbent bulk density, lb/(cu ft)
RH ₀ S (20)	Sorbent particle density, lb/(cu ft)
RH ₀ C (20)	Coolant density, lb/(cu ft)
RH ₀ X (20)	Heat exchanger metal density, lb/(cu ft)
CPG (20)	Specific heat of the process gas, Btu/(1b)(⁰ F)
CPC (20)	Coolant specific heat, Btu/(1b) (⁰ F)
CPX (20)	Heat exchanger specific heat, Btu/({ ⁰ F})(1b)
CPP (20)	Specific heat of dry sorbent, Btu/(1b) (⁰ F)
DX	Axial node dimension, ft
NPSET(3)	Denotes nodes to which vacuum is applied
NDR4	Integer denoting total number of radial sorbent pellet nodes (interior nodes)
NDXMAC	Integer denoting number of active molecular sieve nodes, i.e., (NDXM - NDXMAC) represents the number of molecular sieve nodes which have been inactivated by water poisoning
NBC ₀ UT	Integer control variable; NBC ₀ UT = 1, vacuum duct is simulated; NBC ₀ UT = 2, pressures are set as functions of time at nodes NPSET(1~3); NBC ₀ UT = 3, 4, CO ₂ save system with pump characteristics inputted; fixed volume CO ₂ -accumulator used for NBC ₀ UT = 3, fixed pressure accumulator for NBC ₀ UT = 4
NDXI	Integer denoting total number of axial nodes
NDXM	Integer denoting total number of molecular sieve nodes
N ₀ G	Node to which coolant is added
P ₀ UT (10) TIMET (10)	{ 10 pairs of exit pressure vs time data to be used if NBCOUT = 2; POUT = vacuum end manifold pressures (mm Hg), TIMET = times (hr)



PUMP (10)		10 pairs of pressure ratios vs volumetric displacements to be used for NBCOUT = 3 or 4; PUMP = pump outlet to pump inlet pressure ratio; VPUMP = volumetric displacements, cfm.
VPUMP (10)		
IDSORB (20)		Index identifying sorbent used for each node; 1 = 5A, 2 = S.G., 3 = 13X, 4 = 4A, 5 = 3A.
CPL (2)		Specific heat of adsorbed sorbate, Btu/({°F}) (lb)
DP (20)		Sorbent diameter, ft.

7. Namelist DBA

<u>Fortran Symbol</u>	<u>Definition</u>
HGX (20)	Heat transfer coefficient, heat exchanger to process gas, Btu/(sq ft) ({°F}) (hr)
HXS (20)	Heat transfer coefficient, heat exchanger to sorbent, Btu/(sq ft)(hr)({°F})
HXC (20)	Heat transfer coefficient, heat exchanger to coolant Btu/(sq ft)(hr)({°F})
HSG (20)	Heat transfer coefficient, sorbent to gas, Btu/(hr)(sq ft)({°F})
SK (20)	Effective sorbent thermal conductivity, Btu/(hr) (sq ft) ({°F}/ft)
TKX (20)	Heat exchanger metal thermal conductivity, TKX (K) denotes that between node K-1 and node K, Btu/(hr)(sq ft)({°F}/ft)
DH (20)	Differential heat of adsorption, Btu/(1b adsorbed)
DIF (20)	Internal diffusivity, sq ft/hr
GK (20)	External surface mass transfer coefficient, lb-mol/(hr)(sq ft)(mm Hg)
TCIN	Coolant inlet temperature, {°F}
HTR (20)	Electric heater power for each node, BTU/hr



TMAX Maximum metal temperature, above which heater will be shutt off, °F.

WC Coolant flow rate, lb/hr.

8. Namelist DBD

Parameters characterizing various transfer processes in desorption cycles are contained in this namelist. The list is identical to DBA and will be given below without definition.

HXG (20), HXS(20), HXC(20), HSG(20), SK (20), TKX (20), DH (20),
DIF (20), GK (20), TCIN, HTR (20), TMAX, WC

9. Namelist MB

This namelist comprises the characteristics of CO₂ beds 2 and 4. The list is identical to DB and will be given below without definition.

ABED (20), AVC (20), ASX (20), AGX (20), AXC (20), AVX (20), RHØG (20),
RHØSB (20), RHØS (20), RHØC (20), RHØX (20), GPG (20), CPC (20),
CPX (20), CPP (20), DX, NPSET (3), NDR4, NDXMAC, NBCØUT, NDXI,
NDXM, NØG, PØUT (10), TIMET (10), PUMP (10), VPUMP(10), IDSØRB(20),
CPL (2), DP (20)

10. Namelist MBA

This namelist comprises the data characterizing various transport processes for CO₂ beds 3 and 4 adsorption cycles. The list is identical to DBA and will be given without definition.

HXG (20), HXS (20), HXC (20), HSG (20), SK (20), TKX (20), DH (20),
DIF (20), GK (20), TCIN, HTR (20), TMAX, WC

11. Namelist MBD

This list is equivalent to MBA for desorption cycles.

HXG (20), HXS (20), HXC (20), HSG (20), SK (20), TKX (20), DH (20),
DIF (20), GK (20), TCIN, HTR (20), TMAX, WC

EXECUTION CHARACTERISTICS

Storage Requirement

The present program requires a 28,400 word storage on the Univac 1108 computer.



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Execution Time

With the Univac 1108 computer and using a total of 20 nodes for all four beds, the ratio of real time to computer time is roughly 130 to 1.

Accuracy/Validity

The single bed program S9960 was tested on the regenerable CO₂ removal systems for AAP and Airlock applications and has proved to be quite accurate in performance predictions. It is reasonable to assume that the expanded version, MAIN4B, should be able to predict the performance of a 4-bed-CO₂-H₂O-save system equally well, as the basic models employed in both programs are identical.

Program Limitations

Although the present program was intended to be as general as feasible, the basic system configuration as shown in Figure 6-1 was assumed in writing the main program MAIN4B. Should the coolant hook-up be different from the arrangement depicted in the schematic, the main program must be modified. The work involved should be minimal, however.

Another limitation is that the program uses the built-in equilibrium data of subroutine EQPWT, which represents the best data available at AiResearch at the moment. As better data become available, the subroutine has to be modified. Also pure N₂ and pure O₂ data are employed by the program in estimating overboard gas losses. Should expanded N₂ - O₂ coadsorption data become available, some modifications will be required in the estimation.



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SECTION 9

EXAMPLE RUNS

INTRODUCTION

Two example runs are presented in this section: a performance prediction for a 4-bed- $\text{CO}_2\text{-H}_2\text{O}$ save system; and demonstration of the program to account for the coadsorption of CO_2 with H_2O . Program input and output data are included.

Example run no. 1 is presented on page 144 and example run no. 2 is presented on page 165.



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EXAMPLE RUN NO. 1



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EXAMPLE RUN NO. 1

The first example to be presented is the performance prediction for a 4-bed- $\text{CO}_2\text{-H}_2\text{O}$ save system. This example is very similar to the one shown in Figure 6-1, except that temperature swings of the CO_2 beds are controlled electrically, and an intercooler is used to precool the CO_2 -bed inlet gas stream to 50°F.

Input data required are given as Figure 9-1. These data are printed by the program in the namelist format for input data checking. It should be noted that since no coolant is used in the sorbent beds of the present system, coolant-related data are unimportant for the run. As vacuum dumping is not used for sorbent regeneration, there should be no overboard gas losses, and so $\text{PN}21$, $\text{P}021$, $\text{PN}22$, $\text{P}022$, etc., are set to 10^{-20} . (Setting these to zero causes some problems.)

After the printing of the input data, the program then gives sorbent quantities and estimated gas losses for each bed, as shown in Figure 9-2.

The program is run with $\text{NCT}1=6$ and $\text{NST}1=6$ and printing starts at the 6th cycle. The print-out at the end of the second half of the 6th cycle is presented in Figure 9-3 for all four beds. Beds 3 and 4 have been adsorbing and beds 1 and 2 have been desorbing. A constant pressure type CO_2 -accumulator is used for the system and the accumulator volume at the moment is printed with bed 2 outputs.

Since $\text{NCT}2=0$ for the run, the program stops at this point.

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Figure 9-1. Input Data for Example Run No. 1

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Figure 9-1. (Continued)



Figure 9-1. (Continued)

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Figure 9-1. (Continued.)

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RHOX	=	.00000000+00, .49000000+03, .49000000+03, .49000000+03, .00000000+00, .00000000+00,	.00000000+00, .49000000+03, .49000000+03, .49000000+03, .00000000+00, .00000000+00,	.00000000+00, .49000000+03, .49000000+03, .49000000+03, .00000000+00, .00000000+00,	.00000000+00, .49000000+03, .49000000+03, .49000000+03, .00000000+00, .00000000+00,
CPG	=	.23000000+00, .23000000+00, .23000000+00, .00000000+00, .00000000+00,	.23000000+00, .23000000+00, .23000000+00, .00000000+00, .00000000+00,	.23000000+00, .23000000+00, .23000000+00, .00000000+00, .00000000+00,	.23000000+00, .23000000+00, .23000000+00, .00000000+00, .00000000+00,
CPC	=	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,
CPX	=	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,
CPP	=	.00000000+00, .25000000+00, .25000000+00, .25000000+00, .25000000+00,	.00000000+00, .25000000+00, .25000000+00, .25000000+00, .25000000+00,	.00000000+00, .25000000+00, .25000000+00, .25000000+00, .25000000+00,	.00000000+00, .25000000+00, .25000000+00, .25000000+00, .25000000+00,
DX	=	.25000000+00,	,	,	,
NPSET	=	,	,	,	,
NDR4	=	2,	,	,	,
NDXMAC	=	,	,	,	,
NBCOUT	=	,	,	,	,
NDX1	=	5,	,	,	,
NDXM	=	,	,	,	,
NOG	=	1,	,	,	,
POUT	=	.00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00,
TIMET	=	.00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00,
PUMP	=	.00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00,
VPUMP	=	.00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00,
IDSORB	=	3, 3, 3, 3, 3,	3, 3, 3, 3, 3,	3, 3, 3, 3, 3,	3, 3, 3, 3, 3,
CPL	=	.10200000+01,	.10000000+01,		
DP	=	.64199999-02, .64199999-02, .64199999-02, .64199999-02, .64199999-02, .64199999-02,	.64199999-02, .64199999-02, .64199999-02, .64199999-02, .64199999-02, .64199999-02,	.64199999-02, .64199999-02, .64199999-02, .64199999-02, .64199999-02, .64199999-02,	.64199999-02, .64199999-02, .64199999-02, .64199999-02, .64199999-02, .64199999-02,
SEND					
\$DBA					
HXC	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,

Figure 9-1. (Continued)

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		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
HXS	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
HXC	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
HSG	=	.20000000+02,	.20000000+02,	.20000000+02,	.20000000+02,
		.20000000+02,	.20000000+02,	.20000000+02,	.20000000+02,
		.20000000+02,	.20000000+02,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
SK	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.99999998-01,	.99999998-01,	.99999998-01,
		.99999998-01,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
TKX	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.90000000+01,	.90000000+01,	.90000000+01,
		.90000000+01,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
DH	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
DIF	=	.14000000+04,	.14000000+04,	.14000000+04,	.14000000+04,
		.14000000+04,	.14000000+04,	.14000000+04,	.14000000+04,
		.14000000+04,	.14000000+04,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
GK	=	.40000000-03,	.40000000-03,	.40000000-03,	.40000000-03,
		.40000000-03,	.40000000-03,	.40000000-03,	.40000000-03,
		.40000000-03,	.40000000-03,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
TCIN	=	.10000000-02,	.10000000-02,	.10000000-02,	.10000000-02,
HTR1	=	.10000000-02,	.10000000-02,	.10000000-02,	.10000000-02,
		.10000000-02,	.10000000-02,	.10000000-02,	.10000000-02,
		.10000000-02,	.10000000-02,	.10000000-02,	.10000000-02,
		.10000000-02,	.10000000-02,	.10000000-02,	.10000000-02,
TMAX	=	.40000000+03,			
WCC	=	.00000000+00,			
SEND					
SDBD					
HXG	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
HXS	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,

Figure 9-1. (Continued)



		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
HXC	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
HSG	=	.20000000+02,	.20000000+02,	.20000000+02,	.20000000+02,
		.20000000+02,	.20000000+02,	.20000000+02,	.20000000+02,
		.20000000+02,	.20000000+02,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
SK	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.99999998-01,	.99999998-01,	.99999998-01,	.99999998-01,
		.99999998-01,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
TKX	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.90000000+01,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
DH	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.14000000+04,	.14000000+04,	.14000000+04,	.14000000+04,
		.14000000+04,	.14000000+04,	.14000000+04,	.14000000+04,
		.14000000+04,	.14000000+04,	.00000000+00,	.00000000+00,
DIF	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
GK	=	.40000000-03,	.40000000-03,	.40000000-03,	.40000000-03,
		.40000000-03,	.40000000-03,	.40000000-03,	.40000000-03,
		.40000000-03,	.40000000-03,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
TCIN	=	.10000000-02,	.10000000-02,	.10000000-02,	.10000000-02,
HTR1	=	.10000000-02,	.10000000-02,	.10000000-02,	.10000000-02,
		.10000000-02,	.10000000-02,	.10000000-02,	.10000000-02,
		.10000000-02,	.10000000-02,	.10000000-02,	.10000000-02,
		.10000000-02,	.10000000-02,	.10000000-02,	.10000000-02,
TMAX	=	.40000000+03,			
WCC	=	.00000000+00,			
SEND					
SMB					
ABED	=	.79999999+00,	.79999999+00,	.79999999+00,	.79999999+00,
		.79999999+00,	.79999999+00,	.79999999+00,	.79999999+00,
		.79999999+00,	.79999999+00,	.79999999+00,	.79999999+00,
		.79999999+00,	.79999999+00,	.79999999+00,	.79999999+00,
		.79999999+00,	.79999999+00,	.79999999+00,	.79999999+00,
AVC	=	.52100000+03,	.52100000+03,	.52100000+03,	.52100000+03,
		.52100000+03,	.52100000+03,	.52100000+03,	.52100000+03,
		.52100000+03,	.52100000+03,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
ASX	=	.40000000+02,	.40000000+02,	.40000000+02,	.40000000+02,

Figure 9-1. (Continued)

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		.40000000+02,	.40000000+02,	.40000000+02,	.40000000+02,
		.40000000+02,	.40000000+02,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
AGX	=	.16000000+02,	.16000000+02,	.16000000+02,	.16000000+02,
		.16000000+02,	.16000000+02,	.16000000+02,	.16000000+02,
		.16000000+02,	.16000000+02,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
AVX	=	.32800000+03,	.32800000+03,	.32800000+03,	.32800000+03,
		.32800000+03,	.32800000+03,	.32800000+03,	.32800000+03,
		.32800000+03,	.32800000+03,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
RHOG	=	.30000000-03,	.30000000-03,	.30000000-03,	.30000000-03,
		.30000000-03,	.30000000-03,	.30000000-03,	.30000000-03,
		.30000000-03,	.30000000-03,	.30000000-03,	.30000000-03,
		.30000000-03,	.30000000-03,	.30000000-03,	.30000000-03,
RHOSB	=	.37000000+02,	.37000000+02,	.37000000+02,	.37000000+02,
		.37000000+02,	.37000000+02,	.37000000+02,	.37000000+02,
		.37000000+02,	.37000000+02,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
RHOS	=	.64000000+02,	.64000000+02,	.64000000+02,	.64000000+02,
		.64000000+02,	.64000000+02,	.64000000+02,	.64000000+02,
		.64000000+02,	.64000000+02,	.64000000+02,	.64000000+02,
		.64000000+02,	.64000000+02,	.64000000+02,	.64000000+02,
RHOC	=	.11500000+03,	.11500000+03,	.11500000+03,	.11500000+03,
		.11500000+03,	.11500000+03,	.11500000+03,	.11500000+03,
		.11500000+03,	.11500000+03,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
RHOX	=	.49000000+03,	.49000000+03,	.49000000+03,	.49000000+03,
		.49000000+03,	.49000000+03,	.49000000+03,	.49000000+03,
		.49000000+03,	.49000000+03,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
CPG	=	.23000000+00,	.23000000+00,	.23000000+00,	.23000000+00,
		.23000000+00,	.23000000+00,	.23000000+00,	.23000000+00,
		.23000000+00,	.23000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
CPC	=	.28000000+00,	.28000000+00,	.28000000+00,	.28000000+00,
		.28000000+00,	.28000000+00,	.28000000+00,	.28000000+00,
		.28000000+00,	.28000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
CPX	=	.10999999+00,	.10999999+00,	.10999999+00,	.10999999+00,
		.10999999+00,	.10999999+00,	.10999999+00,	.10999999+00,
		.10999999+00,	.10999999+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
CPP	=	.25000000+00,	.25000000+00,	.25000000+00,	.25000000+00,
		.25000000+00,	.25000000+00,	.25000000+00,	.25000000+00,
		.25000000+00,	.25000000+00,	.25000000+00,	.25000000+00,
		.25000000+00,	.25000000+00,	.25000000+00,	.25000000+00,
		.25000000+00,	.25000000+00,	.25000000+00,	.25000000+00,
DX	=	.25000000+00,	.25000000+00,	.25000000+00,	.25000000+00,

Figure 9-1. (Continued)

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NPSET	=	10,				
NDR4	=	2,				
NDXMAC	=	5,				
NBCOUT	=	4,				
NDX1	=	5,				
NDXM	=	5,				
NOG	=	1,				
POUT	=	.00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00,	
TIMET	=	.00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00,	
PUMP	=	.10000000+01, .25000000+02, .25000000+02,	.25000000+02, .25000000+02, .25000000+02,	.25000000+02, .25000000+02, .25000000+02,	.25000000+02, .25000000+02, .25000000+02,	
VPUMP	=	.30000000+01, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00,	
IDSORB	=	1, 1, 1, 1, 1,	1, 1, 1, 1, 1,	1, 1, 1, 1, 1,	1, 1, 1, 1, 1,	
CPL	=	.10200000+01,	.10000000+01,			
DP	=	.64199999-02, .64199999-02, .64199999-02, .64199999-02, .64199999-02, .64199999-02,	.64199999-02, .64199999-02, .64199999-02, .64199999-02, .64199999-02, .64199999-02,	.64199999-02, .64199999-02, .64199999-02, .64199999-02, .64199999-02, .64199999-02,	.64199999-02, .64199999-02, .64199999-02, .64199999-02, .64199999-02, .64199999-02,	
SEND						
\$MBA						
HXC	=	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,
HXS	=	.96000000+01, .96000000+01, .96000000+01, .00000000+00, .00000000+00,	.96000000+01, .96000000+01, .96000000+01, .00000000+00, .00000000+00,	.96000000+01, .96000000+01, .96000000+01, .00000000+00, .00000000+00,	.96000000+01, .96000000+01, .96000000+01, .00000000+00, .00000000+00,	.96000000+01, .96000000+01, .96000000+01, .00000000+00, .00000000+00,
HXC	=	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,
HSG	=	.50000000+01, .50000000+01, .50000000+01, .00000000+00, .00000000+00,	.50000000+01, .50000000+01, .50000000+01, .00000000+00, .00000000+00,	.50000000+01, .50000000+01, .50000000+01, .00000000+00, .00000000+00,	.50000000+01, .50000000+01, .50000000+01, .00000000+00, .00000000+00,	.50000000+01, .50000000+01, .50000000+01, .00000000+00, .00000000+00,
SK	=	.00000000+00, .99999998-01, .00000000+00, .00000000+00, .00000000+00,	.99999998-01, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.99999998-01, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.99999998-01, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.99999998-01, .00000000+00, .00000000+00, .00000000+00, .00000000+00,
TKX	=	.00000000+00, .90000000+01, .00000000+00,	.90000000+01, .00000000+00, .00000000+00,	.90000000+01, .00000000+00, .00000000+00,	.90000000+01, .00000000+00, .00000000+00,	

Figure 9-1. (Continued)

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DH	=	.00000000+00, .00000000+00, .40000000+03, .40000000+03, .40000000+03, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .40000000+03, .40000000+03, .40000000+03, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .40000000+03, .40000000+03, .40000000+03, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .40000000+03, .40000000+03, .40000000+03, .00000000+00, .00000000+00,
DIF	=	.40000000-04, .40000000-04, .40000000-04, .00000000+00, .00000000+00,	.40000000-04, .40000000-04, .40000000-04, .00000000+00, .00000000+00,	.40000000-04, .40000000-04, .40000000-04, .00000000+00, .00000000+00,	.40000000-04, .40000000-04, .40000000-04, .00000000+00, .00000000+00,
GK	=	.20000000-03, .20000000-03, .20000000-03, .00000000+00, .00000000+00,	.20000000-03, .20000000-03, .20000000-03, .00000000+00, .00000000+00,	.20000000-03, .20000000-03, .20000000-03, .00000000+00, .00000000+00,	.20000000-03, .20000000-03, .20000000-03, .00000000+00, .00000000+00,
TCIN	=	.00000000+00,			
HTR1	=	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,
TMAX	=	.40000000+03,			
WCC	=	.00000000+00,			
\$END					
\$NBD					
HXG	=	.60000000+01, .60000000+01, .60000000+01, .00000000+00, .00000000+00,	.60000000+01, .60000000+01, .60000000+01, .00000000+00, .00000000+00,	.60000000+01, .60000000+01, .60000000+01, .00000000+00, .00000000+00,	.60000000+01, .60000000+01, .60000000+01, .00000000+00, .00000000+00,
HXS	=	.96000000+01, .96000000+01, .96000000+01, .00000000+00, .00000000+00,	.96000000+01, .96000000+01, .96000000+01, .00000000+00, .00000000+00,	.96000000+01, .96000000+01, .96000000+01, .00000000+00, .00000000+00,	.96000000+01, .96000000+01, .96000000+01, .00000000+00, .00000000+00,
HXC	=	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,
HSG	=	.50000000+01, .50000000+01, .50000000+01, .00000000+00, .00000000+00,	.50000000+01, .50000000+01, .50000000+01, .00000000+00, .00000000+00,	.50000000+01, .50000000+01, .50000000+01, .00000000+00, .00000000+00,	.50000000+01, .50000000+01, .50000000+01, .00000000+00, .00000000+00,
SK	=	.00000000+00, .99999998-01, .00000000+00, .00000000+00, .00000000+00,	.99999998-01, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.99999998-01, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.99999998-01, .00000000+00, .00000000+00, .00000000+00, .00000000+00,
TKX	=	.00000000+00, .90000000+01, .00000000+00, .00000000+00, .00000000+00,	.90000000+01, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.90000000+01, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.90000000+01, .00000000+00, .00000000+00, .00000000+00, .00000000+00,
DH	=	.40000000+03, .40000000+03, .40000000+03,	.40000000+03, .40000000+03, .40000000+03,	.40000000+03, .40000000+03, .40000000+03,	.40000000+03, .40000000+03, .40000000+03,

Figure 9-1. (Continued)



DIF	=	.00000000+00, .00000000+00, .40000000-04, .40000000-04, .40000000-04, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .40000000-04, .40000000-04, .40000000-04, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .40000000-04, .40000000-04, .40000000-04, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .40000000-04, .40000000-04, .40000000-04, .00000000+00, .00000000+00,
GK	=	.20000000-03, .20000000-03, .20000000-03, .00000000+00, .00000000+00,	.20000000-03, .20000000-03, .20000000-03, .00000000+00, .00000000+00,	.20000000-03, .20000000-03, .20000000-03, .00000000+00, .00000000+00,	.20000000-03, .20000000-03, .20000000-03, .00000000+00, .00000000+00,
TCIN	=	.00000000+00,			
HTR1	=	.10000000+04, .10000000+04, .10000000+04, .10000000+04, .10000000+04,	.10000000+04, .10000000+04, .10000000+04, .10000000+04, .10000000+04,	.10000000+04, .10000000+04, .10000000+04, .10000000+04, .10000000+04,	.10000000+04, .10000000+04, .10000000+04, .10000000+04, .10000000+04,
TMAX	=	.40000000+03,			
WCC	=	.00000000+00,			
\$END					

Figure 9-1. (Continued)

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BED NO 1

VOLUME AND WEIGHT

BULK VOLUME OF CO ₂ SORBENT (CU FT)	.0000
WEIGHT OF CO ₂ SORBENT (LB)	.0000
WEIGHT OF ACTIVE CO ₂ SORBENT (LB)	.0000
BULK VOLUME OF DESICCANT (CU FT)	1.2500
WEIGHT OF DESICCANT (LB)	56.2500

ESTIMATED CABIN GAS LOSSES

NITROGEN LOSS (LB/HR)	.0000
OXYGEN LOSS (LB/HR)	.0000

Figure 9-2. Sorbent Bed Size and Gas Loss



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BED NO 2

VOLUME AND WEIGHT

BULK VOLUME OF CO ₂ SORBENT (CU FT)	1.0000
WEIGHT OF CO ₂ SORBENT (LB)	37.0000
WEIGHT OF ACTIVE CO ₂ SORBENT (LB)	37.0000
BULK VOLUME OF DESICCANT (CU FT)	.0000
WEIGHT OF DESICCANT (LB)	.0000

ESTIMATED CABIN GAS LOSSES

NITROGEN LOSS (LB/HR)	.0000
OXYGEN LOSS (LB/HR)	.0000

Figure 9-2. (Continued)



BED NO 3

VOLUME AND WEIGHT

BULK VOLUME OF CO ₂ SORBENT (CU FT)	.0000
WEIGHT OF CO ₂ SORBENT (LB)	.0000
WEIGHT OF ACTIVE CO ₂ SORBENT (LB)	.0000
BULK VOLUME OF DESICCANT (CU FT)	1.2500
WEIGHT OF DESICCANT (LB)	56.2500

ESTIMATED CABIN GAS LOSSES

NITROGEN LOSS (LB/HR)	.0000
OXYGEN LOSS (LB/HR)	.0000

Figure 9-2. (Continued)



BED NO 4

VOLUME AND WEIGHT

BULK VOLUME OF CO ₂ SORBENT (CU FT)	1.0000
WEIGHT OF CO ₂ SORBENT (LB)	37.0000
WEIGHT OF ACTIVE CO ₂ SORBENT (LB)	37.0000
BULK VOLUME OF DESICCANT (CU FT)	.0000
WEIGHT OF DESICCANT (LB)	.0000

ESTIMATED CABIN GAS LOSSES

NITROGEN LOSS (LB/HR)	.0000
OXYGEN LOSS (LB/HR)	.0000

Figure 9-2. (Continued)



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80 NO. 1

ADSORPTION CYCLE 6
TIME= 1.60000 HR
96.000 MIN TIME INCREMENT=.01302

AXIAL NODE	PC02, MM	PH2C, MM	GAS TEMP, F	SORBENT TEMP, F	COOLANT TEMP, F	HX CORE TEMP, F
1	2.5782	.0000	112.9449	112.8917	-.0000	.0000
2	2.5782	.0003	119.0301	119.0147	-.0000	.0000
3	2.5782	.0077	120.7881	120.8000	-.0000	.0000
4	2.5782	.2311	119.4347	119.6553	-.0000	.0000
5	2.5782	5.1786	94.2263	94.4383	-.0000	.0000
INLET	2.5782	9.2000	70.0000			

LOADING AT INTERIOR OF SORBENT, LB/LB

SORB NODE	Avg.	1	2	3	4
AXIAL NODE					
1	.0267	.0267	.0267	.0267	.0267
2	.0333	.0333	.0333	.0333	.0333
3	.0389	.0389	.0389	.0389	.0389
4	.0888	.0887	.0887	.0887	.0890
5	.2152	.2152	.2152	.2152	.2154

Avg CO₂ Loading in CO₂ Sorbent (LB/LB)
Time Avg CO₂ Adsorption Rate (LB/HR)
Electrical Heat Input from Start of Cycle (KWH)
Time Avg Outlet PH2O (MM)

Avg H₂O Loading in Desiccant (LB/LB) .0806
 Time Avg H₂O Adsorption Rate (LB/Hr) ,9392
 Heat added by Coolant from Start of Cycle (BTU) .0000

Figure 9-3. Print-Out at End of Six Complete Cycles



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BED NO.	4	ADSORPTION CYCLE	6	96.000 MIN	TIME INCREMENT= .01302 HR		
AXIAL NODE	PCO2, MM	PH2O, MM		GAS TEMP, F	SORBENT TEMP, F	COOLANT TEMP, F	HX CORE TEMP, F
1	.4373	.0000		60.5864	60.7142	-.0000	60.8095
2	.8735	.0000		58.1843	58.3396	-.0000	58.4635
3	1.4763	.0000		55.2669	55.4178	-.0000	55.5300
4	2.0998	.0000		52.4302	52.5273	-.0000	52.6288
5	2.4923	.0000		50.6068	50.6391	-.0000	50.7356
INLET	2.5782	.0000		50.0000			

LOADING AT INTERIOR OF SORBENT, LB/LB							
SORB NODE	Avg	1	2	3	4	5	6
AXIAL NODE							
1	.0120	.0115	.0125				
2	.0210	.0203	.0217				
3	.0334	.0327	.0341				
4	.0454	.0450	.0459				
5	.0540	.0539	.0541				

AVG CO2 LOADING IN CO2 SORBENT (LB/LB) :0332
 TIME AVG CO2 ABSORPTION RATE (LB/HR) :5501
 ELECTRICAL HEAT INPUT FROM START OF CYCLE (KWH) :0000
 TIME AVG OUTLET PH2O (MM) :0000
 AVG H2O LOADING IN DESICCANT (LB/LB) :0000
 TIME AVG H2O ABSORPTION RATE (LB/HR) :0000
 HEAT ADDED BY COOLANT FROM START OF CYCLE (BTU) :0000

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Figure 9-3. (Continued)

BED NO. 1		ADSORPTION CYCLE 6		TIME INCREMENT= .01302 HR	
		TIME= 1.60000 HR	96.000 MIN	PH2O, MM	GAS TEMP, F
AXIAL NODE	PCO2, MM			SORBENT TEMP, F	Coolant Temp, F
1	.4373		.0000	61.7283	61.7383
2	.4373		.0000	65.1308	65.1606
3	.4373		.0000	67.7681	67.7912
4	.4373		.0000	49.6426	49.4840
5	.4373		.0013	31.4529	31.2937
INLET	.4373		.0000	60.5864	

LOADING AT INTERIOR OF SORBENT, LB/LB						
SORB NODE	Avg	1	2	3	4	5
AXIAL NODE						
1	.0263	.0263	.0263			
2	.0329	.0329	.0329			
3	.0375	.0375	.0375			
4	.0624	.0624	.0624			
5	.1114	.1114	.1114			

AVG CO2 LOADING IN CO2 SORBENT (LB/LB)						
TIME AVG CO2 ABSORPTION RATE (LB/HR)						
ELECTRICAL HEAT INPUT FROM START OF CYCLE (KWH)						
TIME AVG OUTLET PH2O (MM)						

.0000 .0541
.0000 .0427
.0000 -1.0427
.0000 .0000
.0000 .0000

TIME AVG H2O ABSORPTION RATE (LB/HR)
HEAT ADDED BY COOLANT FROM START OF CYCLE (BTU) .0000

TIME AVG OUTLET PH2O (MM) 10.2134

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Figure 9-3. (Continued)

BED NO.	2	DESORPTION CYCLE TIME= 1.60000 HR	96.000 MIN	TIME INCREMENT= .01302 HR				
AXIAL NODE		TOTAL PRESS, MM	GAS TEMP, DEG F	SORBENT TEMP, DEG F	Coolant Temp, Deg F	HX CORE TEMP, DEG F		
1		54.2657	390.8997	390.8997	.0000	391.1669		
2		54.2541	405.1958	405.2043	.0000	404.9627		
3		54.2338	404.0395	404.0437	.0000	403.9226		
4		54.2042	395.7084	395.7072	.0000	395.7357		
5		54.1641	389.0017	388.9976	.0000	389.1141		

LOADING AT INTERIOR OF SORBENT					
SORB NODE	Avg	1	2	3	4
AXIAL NODE					
1	.0095	.0096	.0094		
2	.0092	.0093	.0092		
3	.0093	.0094	.0092		
4	.0094	.0095	.0093		
5	.0095	.0096	.0094		

AVG CO ₂ LOADING IN CO ₂ SORBENT (LB/LB)	.0094	AVG H ₂ O LOADING IN DESICCANT (LB/LB)	.0000
TIME AVG CO ₂ DESORPTION RATE (LB/HR)	.5505	TIME AVG H ₂ O ABSORPTION RATE (LB/HR)	.0000
ELECTRICAL HEAT INPUT FROM START OF CYCLE (KWH)	2.1730	HEAT ADDED BY COOLANT FROM START OF CYCLE (BTU)	.0000
ACCUMULATOR CO ₂ PRESSURE (PSIA)	25.0000	CO ₂ ACCUMULATOR VOLUME (CU FT)	2.6784

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Figure 9-3. (Continued)

EXAMPLE RUN NO. 2



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EXAMPLE RUN NO. 2

In the second example, the capability of the program to account for the coadsorption of CO_2 with H_2O is demonstrated. To utilize this capability, the program must be run in two stages. In the first stage, the program is run for NCT1 cycles to establish the amount of water accumulated in a sorbent bed after NCT1 cycles of operation. The quantity of CO_2 -sorbent equivalent to the coadsorption capacity of the desiccant bed is then added to the original CO_2 -sorbent, and the program rerun for NCT2 cycles to obtain the performance of the bed at NCT1 cycles from the beginning, accounting for the coadsorption effect.

In the present example, the Airlock RCRS performance is simulated at 2-days into a mission. The accumulation of H_2O is established by running the program for 96 cycles (half-cycle being 15 minutes), deliberately using an over-sized desiccant section. Pertinent data required for the run are given in Figure 9-4. A total of 18 nodes are used, nine being CO_2 sorbents. The split of sorbents for CO_2 and H_2O is given in Figure 9-5. The program is run for 96 complete cycles (NCT1=96), the coadsorption capacity of the desiccant for CO_2 is calculated at the water loadings prevailing and sorbent bed sizes adjusted accordingly. The new bed sizes are shown in Figure 9-6. The performance of the new bed is then obtained by running the program for 14 complete cycles (NCT2=14). Print-outs at the adsorption and desorption end of the 14th cycle are shown in Figures 9-7 and 9-8. The adsorption half-cycle performance computed by the program is compared with test data (Reference 8) in Figure 9-9. The output P_{CO_2} 's as predicted by the program matches the test results reasonably well; the inlet P_{CO_2} 's as shown are quite different; however, a material balance of the system indicates that the test data are in error, possibly caused by instrumentation line leakage. Figure 9-10 compares the desorption pressures computed by the program with test data. The match is good.



Figure 9-4. Input Data for Example No. 2

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	.10000000-02,	.10000000-02,	.10000000-02,	.10000000-02,
	.10000000-02,	.10000000-02,	.10000000-02,	.10000000-02,
	.10000000-02,	.10000000-02,	.10000000-02,	.10000000-02,
	.10000000-02,	.10000000-02,	.10000000-02,	.10000000-02,
GMRI	= .67000000+02,			
GMW1	= .29500000+02,			
PN21	= .00000000+00,			
PO21	= .00000000+00,			
SEND				
\$B2M				
PA2	= .25800000+03,			
TS02	= .68000000+02,	.68000000+02,	.68000000+02,	.68000000+02,
	.68000000+02,	.70000000+02,	.70000000+02,	.70000000+02,
	.70000000+02,	.70000000+02,	.70000000+02,	.70000000+02,
	.60000000+02,	.50000000+02,	.40000000+02,	.35000000+02,
	.30000000+02,	.20000000+02,	.00000000+00,	.00000000+00,
TC02	= .70000000+02,	.70000000+02,	.70000000+02,	.70000000+02,
	.70000000+02,	.70000000+02,	.70000000+02,	.70000000+02,
	.70000000+02,	.70000000+02,	.70000000+02,	.70000000+02,
	.70000000+02,	.70000000+02,	.65000000+02,	.65000000+02,
	.65000000+02,	.70000000+02,	.00000000+00,	.00000000+00,
TX02	= .68000000+02,	.68000000+02,	.68000000+02,	.68000000+02,
	.68000000+02,	.70000000+02,	.70000000+02,	.70000000+02,
	.70000000+02,	.70000000+02,	.70000000+02,	.70000000+02,
	.60000000+02,	.50000000+02,	.40000000+02,	.35000000+02,
	.30000000+02,	.20000000+02,	.00000000+00,	.00000000+00,
W2	= .23500000-01,	.23500000-01,	.23500000-01,	.23500000-01,
	.24100000-01,	.24100000-01,	.24100000-01,	.24100000-01,
	.23800000-01,	.23800000-01,	.23800000-01,	.23800000-01,
	.23300000-01,	.23300000-01,	.23300000-01,	.23300000-01,
	.22800000-01,	.22800000-01,	.22800000-01,	.22800000-01,
	.22100000-01,	.22100000-01,	.22100000-01,	.22100000-01,
	.29300000-01,	.29300000-01,	.29300000-01,	.29300000-01,
	.29800000-01,	.29800000-01,	.29800000-01,	.29800000-01,
	.30300000-01,	.30300000-01,	.30300000-01,	.30300000-01,
	.39999999-01,	.39999999-01,	.39999999-01,	.39999999-01,
	.39999999-01,	.39999999-01,	.39999999-01,	.39999999-01,
	.49999999-01,	.49999999-01,	.49999999-01,	.49999999-01,
	.49999999-01,	.49999999-01,	.49999999-01,	.49999999-01,
	.49999999-01,	.49999999-01,	.49999999-01,	.49999999-01,
	.49999999-01,	.49999999-01,	.49999999-01,	.49999999-01,
	.49999999-01,	.49999999-01,	.49999999-01,	.49999999-01,
	.69999998-01,	.69999998-01,	.69999998-01,	.69999998-01,
	.20000000+00,	.20000000+00,	.20000000+00,	.20000000+00,
	.20000000+00,	.20000000+00,	.20000000+00,	.20000000+00,
	.56999999-01,	.56999999-01,	.56999999-01,	.56999999-01,
	.56999999-01,	.56999999-01,	.56999999-01,	.56999999-01,
GMR2	= .15500000+02,			
GMW2	= .31000000+02,			
PN22	= .65000000+02,			
PO22	= .19300000+03,			
SEND				
\$B3M				
PA3	= .00000000+00,			
TS03	= .45000000+02,	.45000000+02,	.45000000+02,	.45000000+02,
	.45000000+02,	.45000000+02,	.45000000+02,	.45000000+02,
	.45000000+02,	.45000000+02,	.45000000+02,	.45000000+02,
	.45000000+02,	.45000000+02,	.45000000+02,	.45000000+02,
	.45000000+02,	.45000000+02,	.45000000+02,	.45000000+02,
TC03	= .45000000+02,	.45000000+02,	.45000000+02,	.45000000+02,
	.45000000+02,	.45000000+02,	.45000000+02,	.45000000+02,

Figure 9-4. (Continued)

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		.96000000+01,	.96000000+01,	.96000000+01,	.96000000+01,
		.96000000+01,	.96000000+01,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
HXC	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
HSG	=	.20000000+02,	.20000000+02,	.20000000+02,	.20000000+02,
		.20000000+02,	.20000000+02,	.20000000+02,	.20000000+02,
		.20000000+02,	.20000000+02,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
SK	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.99999998-01,	.99999998-01,	.99999998-01,
		.99999998-01,	.99999998-01,	.99999998-01,	.99999998-01,
		.99999998-01,	.99999998-01,	.00000000+00,	.00000000+00,
TKX	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
DH	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.14000000+04,	.14000000+04,	.14000000+04,	.14000000+04,
		.14000000+04,	.14000000+04,	.14000000+04,	.14000000+04,
		.14000000+04,	.14000000+04,	.00000000+00,	.00000000+00,
DIF	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
GK	=	.49999999-02,	.49999999-02,	.49999999-02,	.49999999-02,
		.49999999-02,	.49999999-02,	.49999999-02,	.49999999-02,
		.49999999-02,	.49999999-02,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
TCIN	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
HTR1	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
TMAX	=	.40000000+03,			
WCC	=	.00000000+00,			
\$END					
\$MB					
ABED	=	.42600000+00,	.42600000+00,	.42600000+00,	.38000000+00,
		.38000000+00,	.38000000+00,	.38000000+00,	.38000000+00,
		.38000000+00,	.42600000+00,	.42600000+00,	.42600000+00,
		.42600000+00,	.42600000+00,	.42600000+00,	.42600000+00,
AVC	=	.42600000+00,	.42600000+00,	.00000000+00,	.00000000+00,
		.10000000+03,	.10000000+03,	.10000000+03,	.10000000+03,
		.10000000+03,	.10000000+03,	.10000000+03,	.10000000+03,
		.10000000+03,	.10000000+03,	.10000000+03,	.10000000+03,
		.10000000+03,	.10000000+03,	.00000000+00,	.00000000+00,
ASX	=	.61799999+01,	.61799999+01,	.61799999+01,	.61799999+01,

Figure 9-4. (Continued)



		.61799999+01,	.61799999+01,	.61799999+01,	.61799999+01,
		.61799999+01,	.61799999+01,	.61799999+01,	.61799999+01,
		.61799999+01,	.61799999+01,	.61799999+01,	.61799999+01,
		.61799999+01,	.61799999+01,	.00000000+00,	.00000000+00,
AGX	=	.61799999+01,	.61799999+01,	.61799999+01,	.61799999+01,
		.61799999+01,	.61799999+01,	.61799999+01,	.61799999+01,
		.61799999+01,	.61799999+01,	.61799999+01,	.61799999+01,
		.61799999+01,	.61799999+01,	.00000000+00,	.00000000+00,
AVX	=	.37500000+03,	.37500000+03,	.37500000+03,	.37500000+03,
		.37500000+03,	.37500000+03,	.37500000+03,	.37500000+03,
		.37500000+03,	.37500000+03,	.37500000+03,	.37500000+03,
		.37500000+03,	.37500000+03,	.37500000+03,	.37500000+03,
RHOG	=	.30000000-03,	.30000000-03,	.30000000-03,	.30000000-03,
		.30000000-03,	.30000000-03,	.30000000-03,	.30000000-03,
		.30000000-03,	.30000000-03,	.30000000-03,	.30000000-03,
		.30000000-03,	.30000000-03,	.30000000-03,	.30000000-03,
RHOSB	=	.43000000+02,	.43000000+02,	.43000000+02,	.36000000+02,
		.36000000+02,	.36000000+02,	.36000000+02,	.36000000+02,
		.36000000+02,	.43000000+02,	.43000000+02,	.43000000+02,
		.43000000+02,	.43000000+02,	.43000000+02,	.43000000+02,
RHOS	=	.43000000+02,	.43000000+02,	.00000000+00,	.00000000+00,
		.64000000+02,	.64000000+02,	.64000000+02,	.64000000+02,
		.64000000+02,	.64000000+02,	.64000000+02,	.64000000+02,
		.64000000+02,	.64000000+02,	.64000000+02,	.64000000+02,
RHOC	=	.11500000+03,	.11500000+03,	.11500000+03,	.11500000+03,
		.11500000+03,	.11500000+03,	.11500000+03,	.11500000+03,
		.11500000+03,	.11500000+03,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
RHOX	=	.49000000+03,	.49000000+03,	.49000000+03,	.49000000+03,
		.49000000+03,	.49000000+03,	.49000000+03,	.49000000+03,
		.49000000+03,	.49000000+03,	.49000000+03,	.49000000+03,
		.49000000+03,	.49000000+03,	.00000000+00,	.00000000+00,
CPG	=	.23000000+00,	.23000000+00,	.23000000+00,	.23000000+00,
		.23000000+00,	.23000000+00,	.23000000+00,	.23000000+00,
		.23000000+00,	.23000000+00,	.23000000+00,	.23000000+00,
		.23000000+00,	.23000000+00,	.23000000+00,	.23000000+00,
CPC	=	.10000000+21,	.10000000+21,	.10000000+21,	.10000000+21,
		.10000000+21,	.10000000+21,	.10000000+21,	.10000000+21,
		.10000000+21,	.10000000+21,	.10000000+21,	.10000000+21,
		.10000000+21,	.10000000+21,	.10000000+21,	.10000000+21,
CPX	=	.10999999+00,	.10999999+00,	.00000000+00,	.00000000+00,
		.10999999+00,	.10999999+00,	.10999999+00,	.10999999+00,
		.10999999+00,	.10999999+00,	.10999999+00,	.10999999+00,
		.10999999+00,	.10999999+00,	.10999999+00,	.10999999+00,
CPP	=	.25000000+00,	.25000000+00,	.25000000+00,	.35100000+00,
		.35100000+00,	.35100000+00,	.35100000+00,	.35100000+00,
		.35100000+00,	.25000000+00,	.25000000+00,	.25000000+00,
		.25000000+00,	.25000000+00,	.25000000+00,	.25000000+00,
DX	=	.55599999-01,			

Figure 9-4. (Continued)



NPSET	=	,		10.	
NDR4	=	2,			
NDXMAC	=	9,			
NBCOUT	=	1,			
NDX1	=	18,			
NDXM	=	9,			
NOG	=	1,			
POUT	=	.11000000+02, .33700000+03, .45000000+02,	.33000000+01, .11700000+03, .34400000+02,	.24500000+03, .82000000+02, .52000000+02,	
TIMET	=	.10000000-04, .30000000+00, .12000000+01,	.20000000-02, .59999999+00, .20000000+01,	.89999998-01, .75000000+00, .19000000+00,	
PUMP	=	.00000000+00, .10000000+04, .25000000+02,	.45000000+00, .25000000+02, .25000000+02,	.50000000+00, .25000000+02, .25000000+02,	
VPUMP	=	.25000000+05, .13000000+05, .00000000+00,	.25000000+05, .00000000+00, .00000000+00,	.13000000+05, .00000000+00, .00000000+00,	
IDSORB	=	1, 1, 1, 3, 3,	1, 1, 1, 3, 3,	1, 1, 1, 3, 3,	
CPL	=	.10200000+01,	.10000000+01,		
DP	=	.64199999-02, .64199999-02, .64199999-02, .64199999-02, .64199999-02,	.64199999-02, .64199999-02, .64199999-02, .64199999-02, .64199999-02,	.64199999-02, .64199999-02, .64199999-02, .64199999-02, .64199999-02,	
\$END					
\$MBA					
HGX	=	.10099999+00, .10099999+00, .10099999+00, .10099999+00, .10099999+00,	.10099999+00, .10099999+00, .10099999+00, .10099999+00, .10099999+00,	.10099999+00, .10099999+00, .10099999+00, .10099999+00, .10099999+00,	.10099999+00, .10099999+00, .10099999+00, .10099999+00, .10099999+00,
HXS	=	.68499999+00, .79500000+02, .79500000+02, .68499999+00,	.68499999+00, .79500000+02, .68499999+00, .68499999+00,	.68499999+00, .79500000+02, .68499999+00, .68499999+00,	.79500000+02, .79500000+02, .68499999+00, .68499999+00,
HXC	=	.68499999+00, .20000000+00, .20000000+00, .20000000+00, .20000000+00,	.20000000+01, .20000000+00, .20000000+00, .69999999+00, .33000000+01,	.00000000+00, .20000000+00, .20000000+00, .33000000+01, .33000000+01,	.00000000+00, .20000000+00, .20000000+00, .33000000+01, .33000000+01,
HSG	=	.20000000+02, .20000000+02, .20000000+02, .20000000+02, .33000000+01,	.20000000+02, .20000000+02, .20000000+02, .20000000+02, .33000000+01,	.20000000+02, .20000000+02, .20000000+02, .00000000+00, .00000000+00,	.20000000+02, .20000000+02, .20000000+02, .20000000+02, .00000000+00,
SK	=	.00000000+00, .11600000+02, .11600000+02, .99999998-01, .99999998-01,	.99999998-01, .11600000+02, .58000000+01, .99999998-01, .99999998-01,	.99999998-01, .11600000+02, .99999998-01, .99999998-01, .99999998-01,	.58000000+01, .11600000+02, .99999998-01, .99999998-01, .99999998-01,
TKX	=	.00000000+00, .90000000+01, .90000000+01,	.90000000+01, .90000000+01, .90000000+01,	.90000000+01, .90000000+01, .90000000+01,	.90000000+01, .90000000+01, .90000000+01,

Figure 9-4. (Continued)

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Figure 9-4. (Continued)

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DTF	=	.140000000+04, .140000000+04, .99999998-04, .99999998-04, .99999998-04, .99999998-04, .99999998-04, .99999998-04, .99999998-04, .99999998-04,	.140000000+04, .140000000+04, .99999998-04, .99999998-04, .99999998-04, .99999998-04, .99999998-04, .99999998-04, .99999998-04, .99999998-04,	.140000000+04, .140000000+04, .99999998-04, .99999998-04, .99999998-04, .99999998-04, .99999998-04, .99999998-04, .99999998-04, .99999998-04,	.140000000+04, .140000000+04, .99999998-04, .99999998-04, .99999998-04, .99999998-04, .99999998-04, .99999998-04, .99999998-04, .99999998-04,	
GK	=	.49999999-03, .49999999-03, .49999999-03, .10000000-02, .10000000-02,	.49999999-03, .49999999-03, .10000000-02, .10000000-02, .10000000-02,	.49999999-03, .49999999-03, .10000000-02, .10000000-02, .10000000-02,	.49999999-03, .49999999-03, .10000000-02, .10000000-02, .10000000-02,	.49999999-03, .49999999-03, .10000000-02, .10000000-02, .10000000-02,
TCIN	=	.00000000+00,				
HTR1	=	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	.00000000+00, .00000000+00, .00000000+00, .00000000+00, .00000000+00,	
TMAX	=	.40000000+03,				
WCC	=	.00000000+00,				
\$END						

Figure 9-4. (Continued)

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BED NO 2

VOLUME AND WEIGHT

BULK VOLUME OF CO ₂ SORBENT (CU FT)	.1978
WEIGHT OF CO ₂ SORBENT (LB)	7.6191
WEIGHT OF ACTIVE CO ₂ SORBENT (LB)	7.6191
BULK VOLUME OF DESICCANT (CU FT)	.2132
WEIGHT OF DESICCANT (LB)	9.1663

ESTIMATED CABIN GAS LOSSES

NITROGEN LOSS (LB/HR)	.0291
OXYGEN LOSS (LB/HR)	.0338

Figure 9-5. Initial Sorbent Bed Size for Example No. 2

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BED NO 2

VOLUME AND WEIGHT

BULK VOLUME OF CO ₂ SORBENT (CU FT)	.2452
WEIGHT OF CO ₂ SORBENT (LB)	9.2227
WEIGHT OF ACTIVE CO ₂ SORBENT (LB)	9.2227
BULK VOLUME OF DESICCANT (CU FT)	.1658
WEIGHT OF DESICCANT (LB)	7.3627

ESTIMATED CABIN GAS LOSSES

NITROGEN LOSS (LB/HR)	.0348
OXYGEN LOSS (LB/HR)	.0395

Figure 9-6. Sorbent Bed Sizes After 2 Days,
Accounting for Coadsorption



AXIAL NODE	PCO ₂ , MM	GAS TEMP, F	SORBENT TEMP, F	COOLANT TEMP, F	WX CORE TEMP, F
1	2,411.7	71.5703	71.5572	69.9997	70.5092
2	2,667.1	72.6753	72.6678	69.9997	70.9539
3	2,941.9	73.3119	73.3130	69.9997	71.7648
4	3,234.8	73.2267	73.2275	69.9997	73.0470
5	3,479.3	73.1696	73.1708	69.9997	73.1090
6	3,368	73.0848	73.0867	69.9997	73.0426
7	4,012.4	72.9480	72.9509	69.9997	72.9147
8	4,292.3	72.7445	72.7484	69.9997	72.7151
9	4,569.9	72.4694	72.4742	69.9997	72.4149
10	4,839.2	72.1309	72.1372	69.9997	71.7272
11	5,185.2	71.6630	71.6666	69.9997	71.1444
12	5,367	71.5102	71.5400	69.9997	70.7924
13	5,367	71.0589	71.0581	69.9997	70.9627
14	5,367	92.9287	92.9268	69.9997	71.5828
15	5,367	108.9492	108.9993	64.9997	71.5795
16	5,367	105.1354	105.3829	64.9997	71.5911
17	5,367	92.2183	92.5228	64.9997	71.5058
18	5,367	9.3505	78.9322	69.9997	72.3010
INLET	5,367	65.0000			

LOADING AT INTERIOR OF SORBENT, LB/LB					
AXIAL NODE	SORB NODE	Avg	1	2	3
1	.0334	.0331	.0336		
2	.0346	.0343	.0349		
3	.0361	.0358	.0364		
4	.0381	.0378	.0385		
5	.0396	.0394	.0402		
6	.0416	.0412	.0420		
7	.0435	.0431	.0440		
8	.0456	.0452	.0460		
9	.0477	.0473	.0481		
10	.0498	.0494	.0502		
11	.0525	.0522	.0528		
12	.0559	.0528	.0529		
13	.1515	.1502	.1508		
14	.1744	.1734	.1755		
15	.1949	.1954	.1984		
16	.2146	.2129	.2144		
17	.2272	.2268	.2276		
18	.2368	.2385	.2391		

TIME AVG CO ₂ ABSORPTION RATE (LB/HR)	AVG CO ₂ LOADING IN CO ₂ SORBENT (LB/LB)	TIME AVG H ₂ O LOADING IN DESICCANT (LB/LB)	AVG H ₂ O LOADING IN COOLANT (LB/LB)	HEAT ADDED BY COOLANT FROM START OF CYCLE (BTU/HR)
0.0233	0.0415	0.2609	0.0419	-0.0070

ELECTRICAL HEAT INPUT FROM START OF CYCLE (BTU/HR) 0.0000
TIME AVG OUTLET PH₂O (MM) 3.4800

TIME AVG H₂O LOADING IN DESICCANT (LB/LB) .3480
TIME AVG H₂O ABSORPTION RATE (LB/HR) -0.0070

Figure 9-7. Print-Out at End of Adsorption Half-Cycle

BED NO. 2

ADSORPTION CYCLE 14
TIME = .25000 HR

15.000 MIN

TIME INCREMENT = .00016 HR



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HEU NO. 2
DESORPTION CYCLE 14
TIME = .25000 HR

TIME INCREMENT = .00368 HR

AXIAL NODE	TOTAL PRESS., MM	GAS TEMP., DEG F.	SORBENT TEMP., DEG F.	COOLANT TEMP., DEG F.	HX CORE TEMP., DEG F.
1	1.7584	68.1609	68.1609	69.9997	68.7299
2	1.7280	67.7145	67.7144	69.9997	68.2275
3	1.7074	66.8417	66.8415	69.9997	67.1297
4	1.6788	65.3593	65.3586	69.9997	65.4254
5	1.6464	63.7844	63.7834	69.9997	63.8385
6	1.6076	62.1667	62.1655	69.9997	62.2322
7	1.5621	60.5090	60.5076	69.9997	60.5112
8	1.5098	58.8138	58.8122	69.9997	58.9089
9	1.4503	57.0026	57.0020	69.9997	57.5127
10	1.3779	55.2448	55.2428	69.9997	60.1886
11	1.3153	53.5110	53.5068	69.9997	62.1856
12	1.2457	51.0611	51.0373	69.9997	64.0047
13	1.1134	49.1168	49.1171	69.9997	65.2500
14	.9735	47.3106	47.3099	69.9997	65.9560
15	.8125	63.6329	63.6350	64.9997	64.6506
16	.6388	52.7621	52.7474	64.9997	62.5547
17	.4522	38.8388	38.8173	64.9997	60.1153
18	.1814	25.2948	25.2663	69.9997	58.3382

LOADING AT INTERIOR OF SORBENT

SORB NODE	Avg	1	2	3	4
AXIAL NODE					
1	.0313	.0316	.0310		
2	.0315	.0318	.0312		
3	.0319	.0322	.0316		
4	.0327	.0330	.0324		
5	.0334	.0337	.0331		
6	.0342	.0345	.0339		
7	.0349	.0352	.0346		
8	.0355	.0358	.0352		
9	.0361	.0364	.0357		
10	.0368	.0369	.0362		
11	.0368	.0372	.0365		
12	.0927	.0927	.0927		
13	.1486	.1489	.1487		
14	.1669	.1691	.1687		
15	.1839	.1842	.1837		
16	.1961	.1964	.1958		
17	.2080	.2083	.2077		
18	.2168	.2168	.2160		

AVG CO₂ LOADING IN CO₂ SORBENT (LB/LB)
TIME AVG CO₂ DESORPTION RATE (LB/HR) .0339
ELECTRICAL HEAT INPUT FROM START OF CYCLE (KW-HR) .2797
ACCUMULATOR CO₂ PRESSURE (PSIA) .0000

AVG H₂O LOADING IN DESCICCANT (LB/LB)
TIME AVG H₂O DESORPTION RATE (LB/HR) .0000
HEAT ADDED BY COOLANT FROM START OF CYCLE (BTU/HOUR) .0000

ACCUMULATOR VOLUME (CU FT) 25.0000
ACCUMULATOR PRESSURE 10.0000

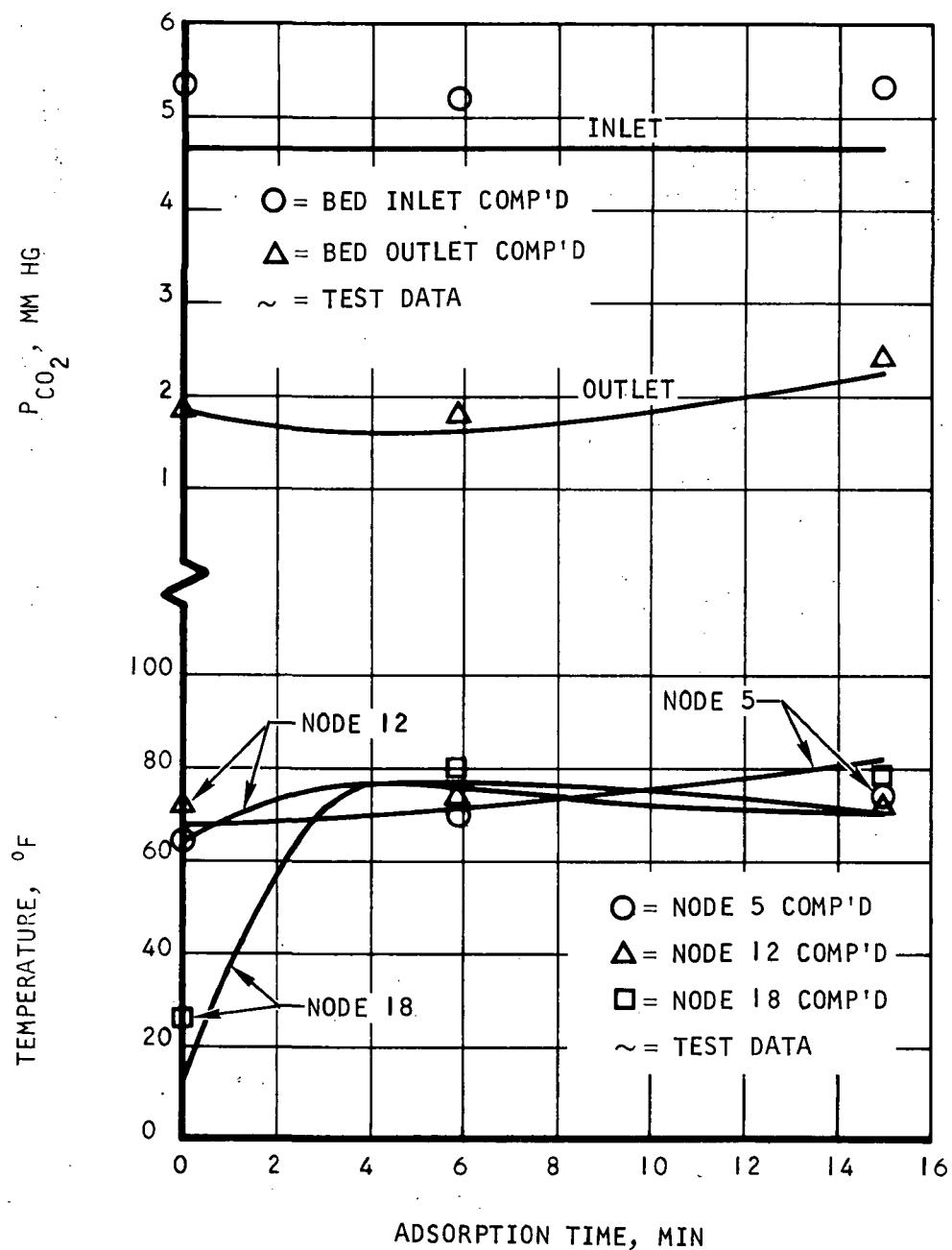
CN₂ ACCUMULATOR VOLUME (CU FT)

ACCUMULATOR PRESSURE 10.0000

Figure 9-8. Print-Out at End of Desorption Half-Cycle



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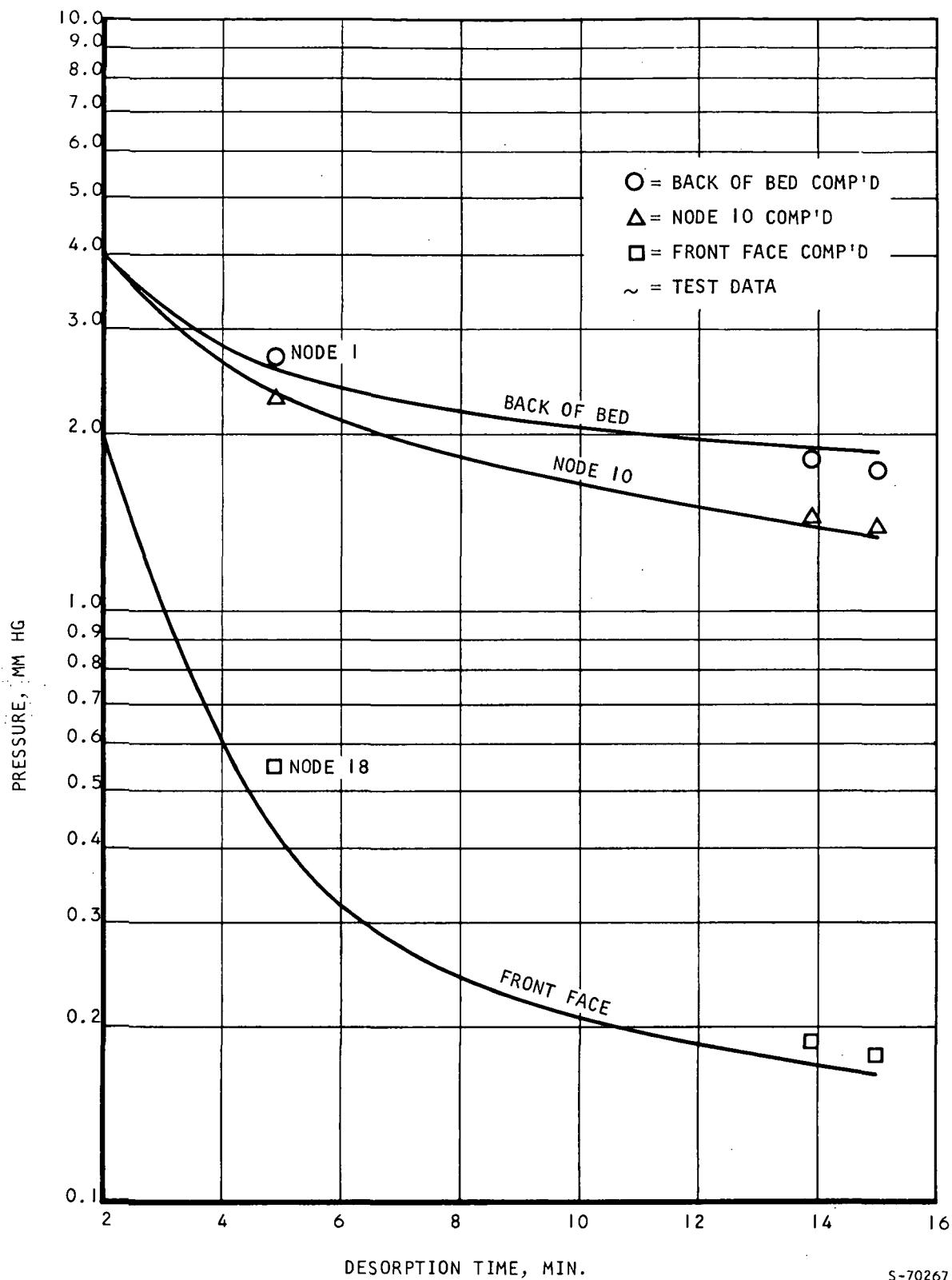
S-70266

Figure 9-9. Comparison of Computed Adsorption Cycle Performance with Test Data (Cycle 94 of 28 Day Test); Lines

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Figure 9-10. Comparison of Computed Desorption Pressures with Test Data (Cycle 94 of 28 Day Test)

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APPENDIX A

SUBPROGRAM DOCUMENTATION



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APPENDIX A

SUBPROGRAM DOCUMENTATION

This appendix contains descriptions of newly developed subprograms for program MAIN4B. The reader is referred to the original single bed program S9960 (Part I of this report) for the description of the old subprograms.

ADSØRB

Adsorption/gas stripping subroutine. Refer to Part I of this report.

BED4

The creation of this subroutine was necessitated by the impracticability of transferring all the bed data required in various subroutines, from one subroutine to another. There are a maximum of four beds in the system, and these data must be stored in different locations. A primary function of BED4 is to transfer the bed data stored under dummy bed variables RDB, IDB, RMB, etc., to the actual variables used in adsorption/desorption subroutines, such as TG, ABED, etc., and vice versa. A logic diagram of BED4 is given in Figure A-1. It is apparent that, in addition to storage transfers, the subroutine controls various options and printouts.

DESØRB

This subroutine performs vacuum desorption calculations and is an expanded version of the original subroutine S9983.

The new version uses a more generally applicable analysis of the vacuum duct, and for a CO_2 -save system, vacuum pump characteristics can be inputted.

EQPWT

This is a new equilibrium data subroutine, which uses a two dimensional interpolation scheme to find the equilibrium pressure or loading corresponding respectively to a given set of loading and temperature or pressure and temperature. Arguments of the subroutine are:

ID = Index identifying sorbate, 1 for CO_2 , 2 for H_2O , 3 for N_2 ,
4 for O_2 .

IDSØRB = Index identifying sorbent, 1 for 5A, 2 for S.G., 3 for 13X,
4 for 4A, 5 for 3A.

KPW = Control index, 1 to find P, given W and T, 2 to find W,
given P and T.

P = Vapor pressure of sorbate, mm Hg.



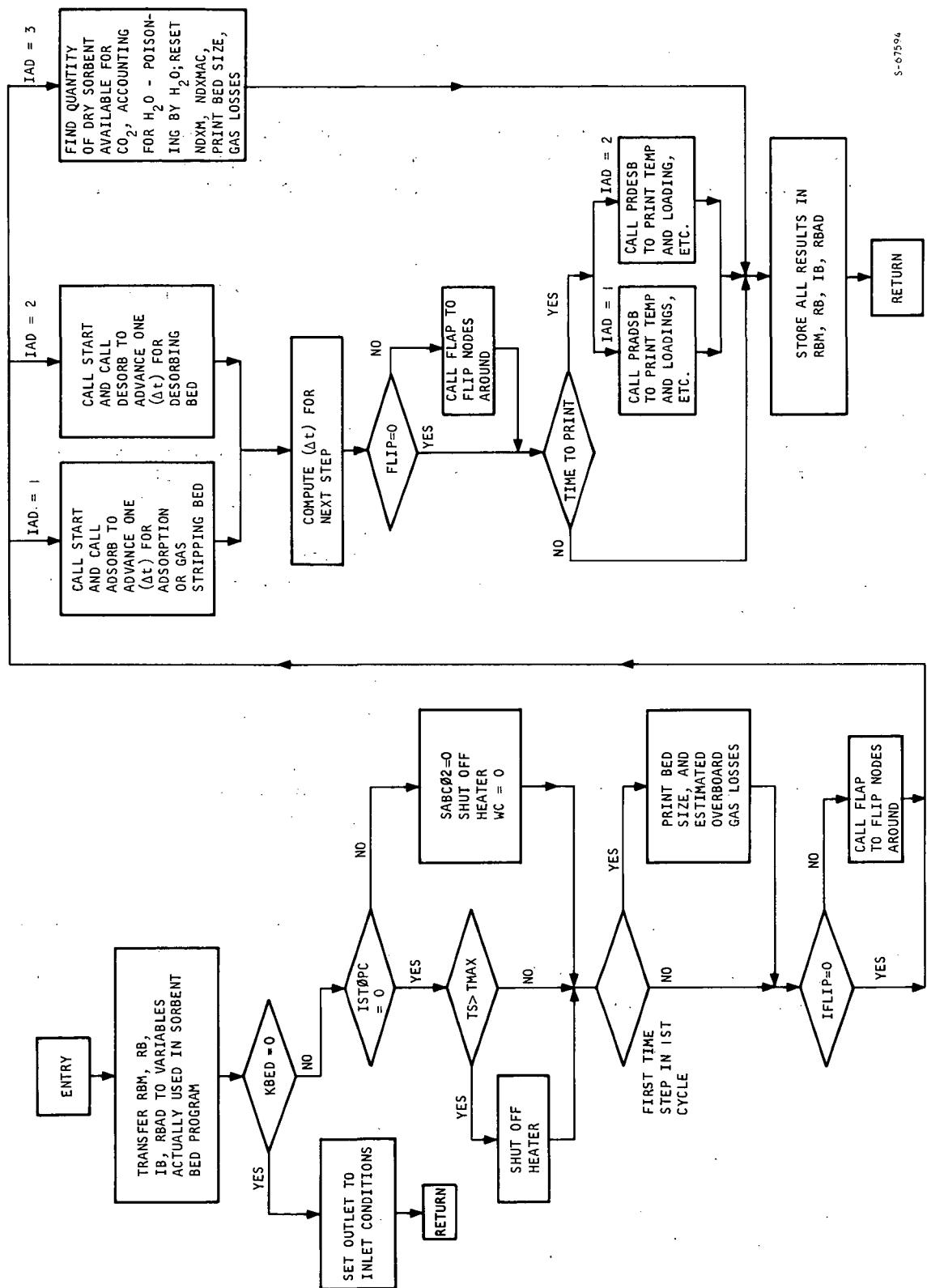


Figure A-1. Logic Diagram for Subroutine BED4

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S-67594

W = Loading, (lb sorbate)/(lb dry sorbent)

T = Temperature, °F

The equilibrium data currently available for various sorbate-sorbent systems are stored in the subroutine in the form of data statements. The variable names used for these data are:

TTAB (NT(IS),IS) = Temperature, °F

WTAB (K,NT(IS),IS) = Loading, (lb sorbate)/(lb dry sorbent)

PTAB (K,NT(IS),IS) = vapor pressure, mm Hg

NT (IS) = Number of temperatures at which W versus P are tabulated for IS system

IDSMTX (IDSØRB, ID) = A two-dimensional array which tabulates IS for each combination of IDSØRB and ID; refer to Table A-1.

FCØAD

This function subprogram determines fractional effectiveness of partially water-poisoned sorbents for CO_2 adsorption by table look-ups.

The coadsorption data are stored as FCØADT (I, IDSØRB) versus H2ØT(I), I = 1 to I2.

FDEQID

No changes made; refer to Part I of this report.

FDEQIM

Same; refer to Part I of this report.

FLAP

This subroutine switches bed properties around; node 1 interchanges with node NDX1, node 2 interchanges with node (NDX1-1), and so forth. This is required when the gas flow direction is reversed as is the case where gas stripping is used to regenerate a bed.

FLIP

A subroutine used by FLAP.

FLØP

A subroutine used by FLAP.



TABLE A-1

TABULATION OF IS FOR EACH
COMBINATION OF IDSORB AND ID

^{ID} ^{IDSORB} ^{IS}	1 (CO ₂)	2 (H ₂ O)	3 (N ₂)	4 (O ₂)	5
1 (5A)	1	2	6	7	
2 (S.G.)		3			
3 (13X)	4	5	8	9	
4 (4A)					
5 (3A)					

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GAST

Refer to Part I of this report.

GASTA

Refer to Part I of this report.

HXCØRE

Same as HXCØRE in the original program except that it now solves Equation (4), which has a source term to account for the heater output.

IFN

Refer to Part I of this report.

LAGIN2

Refer to Part I of this report.

NEWTØ2

An iteration routine using the Newton-Wegstein method.

Arguments of the subroutine are:

NI = Control index indicating the total number of iterations made;
NI should be set equal to 1 before NEWTØ2 is called.

NGØ = Output index; 1 for conversion still unreached, 2 for
conversion reached

X = Independent variable; value of X to be found such that Y = 0.

Y = Dependent variable, which should approach zero as a conversion
is attained.

X0 = Previous value of X.

Y0 = Previous value of Y.

XMIN = Minimum limit for X.

XMAX = Maximum limit for X.

ER = Conversion criterion. If $|Y| < ER$ conversion has been reached.

PRADSB

Refer to Part I of this report.



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PRDESB

Refer to Part I of this report.

PRDESB

Refer to Part I of this report.

READ1

The subroutine reads in namelists 'DB' and 'DBA'.

READ2

The subroutine reads in namelist 'DBD'.

READ3

The subroutine reads in namelists 'MB' and 'MBA'.

READ4

The subroutine reads in namelist 'MBD'.

START

This is a subroutine to replace the original START and STARTA.

TGLCØL

Refer Part I of this report.

TSØRB

Refer to Part I of this report.

TSØRBA

Refer to Part I of this report.

XYZMAP

This is a two-dimensional interpolation routine. The argument variables are:

IND = Option index; IND = 0, Z = F(X,Y); IND = 1, Y = F(X,Z); IND = -1, Y = F(X).

X,Y,Z = Independent and dependent variables.

NP = Number of points per curve, or number of X,Y pairs for each Z.



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NC = Number of curves, i.e., number of Z-values.

IDX = Number of data points to be used in interpolating in X - direction.

IDY = Number of data points to be used in interpolating in Y - direction.

BX = First independent variable.

BY = Second independent variable.

ANS = Dependent variable found corresponding to BX, BY. In another word, = XYZMAP.



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APPENDIX B

PROGRAM LISTING



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APPENDIX B
PROGRAM LISTING

This appendix contains a total listing of program MAIN4B.

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* ELT ADSORB, 1, 710719, 62333 , 1

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000001      SUBROUTINE ADSORB
000002      COMMON/AD/ TG(20),PH20I,TGI,PA,          PK(2,20),PC02I,TS(20)      *NEW
000003      1,TC(20),TX(20),TS1(20),TS2(20),TX1(20),TX2(20),TC1(20),      *NEW
000004      2TC2(20),W(4,20),PT(20),          GMR,GMW,GVIS,PN2,P02,      *NEW
000005      3,ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),      *NEW
000006      4AVX(20),RHOC(20),RHOS9(20),RHOS(20),RHOC(20),RHOX(20),      *NEW
000007      5CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),      *NEW
000008      6POUT(10),TIMET(10),WTACMS,WTSG,PUMP(10),VPUMP(10),CPP(20),      *NEW
000009      7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20),      *NEW
000010      8,HXG(20),HXS(20),HXC(20),HSG(20),      *NEW
000011      9SK(20),TKX(20),DH(20),DJF(20),GK(20),UC(20),T268,TOTCO2,TOTH20,      *NEW
000012      1SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX,      *NEW
000013      1TOTKWH,HTR1(20),WC,TOTHTC,WCC,PC02A,VC02A,SABC02,TC02A,      *NEW
000014      1RS1(2U,9),          A(20),F(20),C(20),VS(20),DVS(20),RS(20),      *NEW
000015      1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),      *NEW
000016      2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),      *NEW
000017      3FR(2,20),          P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3      *NEW
000018      4(20,4),          C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20).      *NEW
000019      5,WM(2),TIME,CYCLE,DTO,          DTMAX,WI,TI,PC02C,      *NEW
000020      6VOLCAB,RC02C,      *NEW
000021      7NCYCLT,NPRINT,NCYCLE,NDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SABC05      *NEW
000022      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,      *NEW
000023      1,CP1,CP2,X,          C1P,C2P,C3P,D1P      *NEW
000024      DIMENSION AS(20)      *NEW
000025      EQUIVALENCE (ASX,AXS),(AGX,AXG),(ASG,AGS),(HXS,HSK),(HXG,HGX),(HSG      *NEW
000026      1,HGS)
000027      DATA RGAS/554./
000028
000029      C
000030      NDR=NDR4-1
000031      DO 21 N=1,NDX1
000032      AS(N)=4.*3.1416*RS(N)**2
000033      I=N
000034      DO 20 NR=1,NDR4
000035      C1(NR,N)=CR2(I,NR)
000036      C2(NR,N)=CR1(I,NR)/DT+CR2(I,NR)+CR3(I,NR).
000037      20 C3(NR,N)=-CR3(I,NR)
000038      C
000039      B(1,N)=C3(1,N)/C2(1,N)
000040      DO 21 J=2,NDR
000041      21 B(J,N)=C3(J,N)/(C2(J,N)-C1(J,N)*B(J-1,N))
000042      NDX=NDX1-1
000043      C TO TEMPORARILY STORE SURFACE LOADING
000044      DO 50 N=1,NDX1
000045      50 WS(N)=W(NDR4,N)
000046      IF (NTEMP.EQ.0) GO TO 111
000047      C
000048      TO CALCULATE CS1,CS2,DS FOR SORBENT HEAT BALANCE EQUATION
000049      DO 12 N=1,NDX1
000050      I=IFN(N,NDXM)
000051      CS2(N)=DT/CPS(N)/RHOS9(N)*ASG(N)*GK(N)*WM(I)*DH(N)
000052      CS1(N)=CS2(N)
000053      IF (N.EQ.1) GO TO 13
000054      IF (N.EQ.NDX1) GO TO 14
000055      S1=SK(N)/DX**2*(TS(N-1)-2.*TS(N)+TS(N+1))
000056      GO TO 15
000057      13 S1=SK(1)/DX**2*(TS(2)-TS(1))
000058      GO TO 15

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000059      14 S1=SK(NDX1)/DX*2*(TS(NDX)-TS(NDX1))
000060      15 DS(N)=DT/CPS(N)/RHOSB(N)*(S1+ASG(N)*HSG(N)*(TG(N)-0.5*TS2(N))+*
000061          1ASX(N)*HXS(N)*(TX(N)-0.5*TS2(N)))
000062          RATIO = (DT+DTO)/DT
000063          T=(DT+DTO)/CPS(N)/RHOSB(N)
000064          T1=0.5*T*(ASG(N)*HSG(N)+ASX(N)*HXS(N))
000065          CS1(N)=RATIO*CS1(N)/(1.+T1)
000066          CS2(N)=RATIO*CS2(N)/(1.+T1)
000067          DS(N)=RATIO*DS(N)
000068          DS(N)=(DS(N)-T1*TS2(N))/(1.+T1)
000069      12 CONTINUE
000070      GO TO 110
000071      111 DO 112 N= 1, NDX1
000072          CS1(N)=0.
000073          CS2(N)=0.
000074          DS(N)=0.
000075          TS(N)=T268
000076          TC(N)=T268
000077          TX(N)=T268
000078          TG(N)=T268
000079      112 CONTINUE
000080      110 CONTINUE
000081
000082      C   TO CALCULATE PARTIAL PRESSURE OF ADSORBATE IN GAS STREAM
000083      C
000084      DO 24 N=1,NDX1
000085      I=IFN(N,NDXM)
000086      C   TO CALCULATE P1,P2,P3
000087      WSURF=W(NDR4,N)
000088      CALL EQPWT(I,IDSORB(N),1,PSURF,WSURF,TS2(N))
000089      CALL EQPWT(I,IDSORB(N),1,PS1,    WSURF,(TS2(N)+0.02))
000090      DPKDTS=(PS1-PSURF)/0.02
000091      CALL EQPWT(I,IDSORB(N),1,PS2,(WSURF+1.E-5),TS2(N))
000092      DPKDWK=(PS2-PSURF)/1.E-5
000093      G=1.+CS2(N)*DPKDTS
000094      P1(N)=(PSURF           +DS(N)*DPKDTS)/G
000095      P2(N)=DPKDWK/G
000096      P3(N)=CS1(N)/G*DPKDTS
000097      C
000098      C2(NDR4,N)=CR1(N,NDR4)/DT+CR2(N,NDR4)+WM(I)*GK(N)*P2(N)*AS(N)
000099      C3(NDR4,N)=0.0
000100      DO 23 NR=1,NDR4
000101      2.3 D1(NR,N)=CR1(N,NR)/DT*W(NR,N)
000102      D1(NDR4,N)=D1(NDR4,N)-WM(I)*GK(N)*(P1(N)-P2(N)*W(NDR4,N))*AS(N)
000103      D2(N)=AS(N)*WM(I)*GK(N)*( 1.          -P3(N))
000104      D2(N)=D2(N)/(C2(NDR4,N)-C1(NDR4,N)*B(NDR4-1,N))
000105      Q(1,N)=D1(1,N)/C2(1,N)
000106      DO 24 J=2,NDR4
000107      24 Q(J,N)=(D1(J,N)-C1(J,N)*Q(J-1,N))/(C2(J,N)-C1(J,N)*B(J-1,N))
000108      C
000109      DO 25 N=1,NDX1
000110      I=IFN(N,NDXM)
000111      CP1(N)=ASG(N)*GK(N)*(P1(N)+P2(N)*(Q(NDR4,N)-W(NDR4,N)))
000112      25 CP2(N)=ASG(N)*GK(N)*(P2(N)*D2(N)+P3(N)-1.0)
000113      PK(1,NDX1+1) = PC02I
000114      PK(2,NDX1+1) = PH20I
000115      DO 26 N=1,NDX1
000116          N1=NDX1+1-N
000117          I=IFN(N1,NDXM)
000118          PK(I,N1) = (PK(I,N1+1)/DX+CP1(N1)/A(N1))

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000119      1          /(1./DX-CP2(N1)/A(N1))
000120      IF ( I.EQ.1)J=2
000121      IF(I.EQ.2)J=1
000122      PK(J,N1)=PK(J,N1+1)
000123 26. CONTINUE
000124      C
000125      C
000126      C
000127      C      TO CALCULATE SORBENT LOADING
000128      C
000129      DO 30 N=1,NDX1
000130      I=IFN(N,NDXM)
000131      W(NDR4,N)=Q(NDR4,N)+D2(N)*PK(I,N)
000132      DO 30 J=2,NDR4
000133      L=NDR4+1-J
000134      30 W(L,N)=Q(L,N)+B(L,N)*W(L+1,N)
000135      C
000136      C
000137      IF( NTEMP .EQ. 0) RETURN
000138      C      TO CALCULATE SORBENT, GLYCOL, HX CORE AND GAS TEMPERATURES
000139      C
000140      CALL TSCRBA
000141      CALL TGLCOL(TC,NDX1,UC,RHOC,CPC,CX,AXC,HXC,T268,TX,DX,DT,
000142      1AVC, NOG ,DTO,TS1,TS2,TX1,TX2,TC1,TC2)
000143      CALL HXCORE
000144      CALL GASTA(GMR,CPG,ABED,NDX1,TG1,ASG,HSG,AXG,HXG,DX,TG,TS,TX)
000145      RETURN
000146      END

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* ELT BED4,1,710720, 31270 , 1

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0J0001      SUBROUTINE BED4(IBED,IFLIP,IAD,RBM,RB,IB,RBAD,ISTOPC,KBED)
0J0002      COMMON/AD/   TG(20),PH20I ,TGI ,PA ,          PK,(2,20),PC02I ,TS (20)
0J0003      1,TC (20),TX (20), TS1 (20),TS2 (20),IX1 (20),TX2 (20),TC1 (20),
0J0004      2TC2 (20),W (4,20),PT (20),          GMR ,GMW,GV16, PN2,P02,
0J0005      3          ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),
0J0006      4AVX(20),RHOG(20),RHOS(20),RHOS(20),RHOC(20),RHOX(20),
0J0007      5CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),
0J0008      6P0UT(10),TIMET(10),WTACMS,WTSG ,PUMP(10),VPUMP(10),CPP(20),
0J0009      7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20),
0J0010      8          HXG(20),HXS(20),HXC(20),HSG(20),
0J0011      9SK(20),TKX(20),DH(20),DJF(20),GK(20),UC(20),T268,TOTCO2,TOTH20,
0J0012      1SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX,
0J0013      1 TOTKWH,HTR1(20),WC,TOTHTC,WCC,PC02A,VC02A,SABC02, TCO2A,
0J0014      1RS1(20,9), A(20),F(20),C(20),VS(20),DVS(20),DVS1(20),RS(20),
0J0015      1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),
0J0016      2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),
0J0017      3FR(2,20), P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3
0J0018      4(20,4), C3(4,20),B1(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20),
0J0019      5 WM(2),TIME,CYCLE,DTO, DTMAX,WI,TI,PC02C,
0J0020      6VOLCAB,RC02C,
0J0021      7NCYCLT,NPRINT,NCYCLE,VDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SABC0S
0J0022      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,
0J0023      1 CP1,CP2,X, C1P,C2P,C3P,D1P
0J0024      DIMENSION RBM(1), RB(1), IB(1), RBAD(1),KRED(1)
0J0025      DIMENSION WN(20)
0J0026      C IFLIP =0, NO FLIP, IFLIP=1, FLIP WILL BE CALLED
0J0027      DATA ISTART/0/
0J0028      C
0J0029      DO 110 N=1,349
0J0030      110 TG(N)=RBM(N)
0J0031      D0111 N=1, 405
0J0032      111 ABED(N)=RB(N)
0J0033      D0112 N= 1,29
0J0034      112 NPSET(N)=IB(N)
0J0035      D0 13 N=1,251
0J0036      13 HXG(N)=RBAD(N)
0J0037      IF(KBED(IBED),EQ, 0) GO TO 90
0J0038      8976 FORMAT(I25)          * THESE TWO CARDS ARE ENTROPY GENERATORS
0J0039      NDX10=NDX1
0J0040      NDX1=NDX10
0J0041      SABC02=SABC0S
0J0042      IF(ISTOPC .NE. 0) SABC02=0.0
0J0043      D0 1311 N= 1, NDX1
0J0044      HTR(N)=HTR1(N)
0J0045      IF(ISTOPC .NE. 0) GO TO 3198
0J0046      IF(TS(N) .GT. TMAX) GO TO 3198
0J0047      GO TO 1311
0J0048      3198 D0 411 J= 1, NDX1
0J0049      411 HTR(J) = 0.0
0J0050      GO TO 66
0J0051      1311 CONTINUE
0J0052      66 CONTINUE
0J0053      ISTART=ISTART+1
0J0054      IF(TIME .LT. 1.1E-5) GO TO 80
0J0055      GO TO 81
0J0056      80 SUMPTM=0.0
0J0057      TOTKWH=0.0
0J0058      TOTCO2=0.0

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000059      TOTHTC=0.
000060      TOTHTC=0.
000061      IF(ISTART .GT. 4) GO TO 81
000062      C
000063          ASSIGN 82 TO NPRSBR
000064          GO TO 183
000065      82 CONTINUE
000066      C
000067          81 WC=WCC
000068              IF(ISTOPG.NE.0) WC=0
000069              DO 801 N=1,NDX1
000070                  AC=ABED(N)*ASX(N)/AVC(N)
000071                  UC(N)=WC/AC/RHOC(N)
000072                      IF(IFLIP.NE.0) CALL FLAP
000073                      15 GO TO (16,17,18), IAD
000074                      16 CALL START
000075                          CALL ABSORB
000076                          SUMPTM= SUMPTM+PK(2,1)*DT
000077                          GO TO 19
000078                      17 CALL START
000079                          CALL DESORB
000080                      19 ADT = DTMAX
000081                      DO 60 N=1,NDX1,4
000082                          ADT2=WI / (ABS(W(N)DR4,N)-WS(N))+1.E-9)*DT
000083                          IF(ADT2.LT. ADT) ADT=ADT2
000084                          ADT2=T1/(ABS( TS(N)-TS2(N))+1.E-9)*DT*2.0
000085                          IF(ADT2.LT. ADT) ADT=ADT2
000086                          ADT2=T1/(ABS( TX(N)-TX2(N))+1.E-9)*DT*2.0
000087                          IF(ADT2.LT. ADT) ADT=ADT2
000088                          ADT2=T1/(ABS( TC(N)-TC2(N))+1.E-9)*DT*2.0
000089                          IF(ADT2.LT. ADT) ADT=ADT2
000090      60 CONTINUE
000091          IF(ADT.LT. 1.E-5) ADT=1.E-5
000092          DTT(IBED)=ADT
000093          DO 21 N=1,NDX1
000094              TS2(N)=TS1(N)
000095              TS1(N)=TS(N)
000096              TX2(N)=TX1(N)
000097              TX1(N)=TX(N)
000098              TC2(N)=TC1(N)
000099              TC1(N)=TC(N)
000100      21 CONTINUE
000101          IF(IFLIP .NE. 0) CALL FLAP
000102          DO 211 N= 1, NDX1
000103              TOTKWH=TOTKWH+DT*HTR(N)/3410.
000104              TOTHTC=TOTHTC+WC*CPC(VOG)*DT*(T268-TC(NDX1))
000105              IF(
000106                  ((TIME.LT.1.E-5).OR.(TIME.GE.CYCLE);OR. (NPR/NPRINT*NPRINT
000107                  2.EQ.NPR)).AND. (NCYCLE.GE. NSTART)) GO TO 130
000108              GO TO 33
000109      130 CONTINUE
000110          GO TO(131,32), IAD
000111      131 CALL PRADSB(IBED)
000112          GO TO 33
000113      32 CALL PRDESB(IBED)
000114          GO TO 33
000115      33 DO 20 N=1,349
000116          20 RBM(N)=TG(N)
000117          DO 23 N=1,251
000118          23 RBAD(N)=HXG(N)

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000119      DO 41 N= 1, 405
000120      41 RB(N)=ABED(N)
000121      DO 181 N=1,29
000122      181 IH(N)=NPSET(N)
000123      RETURN
000124      18 SUMCOS=0.
000125      IF(NDXM.EQ.NDX1)CALL EXIT
000126      NDB=NDXM+1
000127      DO 42 N=NDB,NDX1
000128      CALL EQPWT(1,IDSORB(N),2,3.,WN1,70.)
000129      WN(N)=WN1*ABED(N)*DX*RHOSB(N)
000130      SUMCOS=SUMCOS+WN(N)*FCOAD(IDSORB(N),W(1,N))
000131      42 CONTINUE
000132      DO 43 N=NDB,NDX1
000133      DIF(N)=DIF(1)
000134      GK(N)=GK(1)
000135      DH(N)=DH(1)
000136      IF(SUMCCS-WN(N))46,44,44
000137      46 CONTINUE
000138      FRHO=SUMCOS/WN(N)
000139      DRHO=RHOSB(N)*(1.-FRHO)
000140      RHOSB(N)= RHOSB(N)*FRHO
000141      IF(N.LT.NDX1) GO TO 51
000142      RHOSB(N+1)=DRHO
000143      GO TO 50
000144      51 NTDB=NDX1-N
000145      DRHO1=DRHO/NTDB
000146      K1=N+1
000147      DO 53 K=K1,NDX1
000148      53 RHOSB(K)=RHOSB(K)+DRHO1
000149      50 NDXM=N
000150      NDXMAC=N
000151      ASG(N)=ASG(1)*RHOSB(N)/RHOSB(1)
000152      IF(N.EQ.NDX1)NDX1=NDX1+1
000153      GO TO 47
000154      44 SUMCOS=SUMCOS-WN(N)
000155      ASG(N)=ASG(1)*RHOSB(N)/RHOSB(1)
000156      IF(SUMCOS.LT.1,E-10) GO TO 50
000157      43 CONTINUE
000158      47 CONTINUE
000159      49 CONTINUE
000160      ASSIGN 83 TO NPRSBR
000161      GO TO 183
000162      83 CONTINUE
000163      GO TO 33
000164      90 CONTINUE
000165      PK(1,1)=PC02I
000166      91 PK(2,1)=PH20I
000167      TG(1)=TGI
000168      GO TO 33
000169      C
000170      C
000171      C PRSBWT ROUTINE    CCCCCCCCCC
000172      183 CONTINUE
000173      WCC=WC
000174      N1=NDXM+1
000175      VMS = 0.0
000176      WTMS=0.0
000177      VSG=0.0
000178      WTSG=0.0

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000179      IF(NDXM .EQ. 0) GO TO 11
000180      DO 10 N= 1, NDXM
000181      VMS=VMS+DX*ABED(N)
000182      WTMS=WTMS+DX*ABED(N)*RHOSB(N)
000183      10 CONTINUE
000184      11 CONTINUE
000185      IF((NDX1-NDXM) .EQ. 0) GO TO 31
000186      DO 30 N= N1, NDX1
000187      VSG=VSG+DX*ABED(N)
000188      WTSG=WTSG+DX*ABED(N)*RHOSB(N)
000189      30 CONTINUE
000190      31 CONTINUE
000191      WTACMS=0.0
000192      WN2L=0.0
000193      W02L=0.0
000194      TN2=70.
000195      T02=70.
000196      IF(NDXMAC .EQ. 0) GO TO 12
000197      DO 70 N= 1, NDXMAC
000198      CALL EQPWT(3,IDSORB(N),2,PN2,WN2,TN2)
000199      CALL EQPWT(4,IDSORB(N),2,P02,W02,T02)
000200      WN2L=WN2L+DX*ABED(N)*RHOSB(N)*WN2
000201      W02L=W02L+DX*ABED(N)*RHOSB(N)*W02
000202      70 WTACMS=WTACMS + DX*ABED(N)*RHOSB(N)
000203      12 CONTINUE
000204      WRITE(6,503) IBED
000205      503 FORMAT(1H1//7H BED NO I2/// 20H VOLUME AND WEIGHT // )
000206      WRITE(6,500) VMS,WTMS,WTACMS,VSG,WTSG
000207      500 FORMAT(
000208      1' BULK VOLUME OF CO2 SORBENT (CU FT) 'F8.4/
000209      2' WEIGHT OF CO2 SORBENT (LB) 'F8.4/
000210      3' WEIGHT OF ACTIVE CO2 SORBENT (LB) 'F8.4//'
000211      4' BULK VOLUME OF DESICCANT (CU FT) 'F8.4/
000212      5' WEIGHT OF DESICCANT (LB) 'F8.4)
000213      C
000214      CALL START
000215      WN2V=0.
000216      W02V=0.0
000217      DO 600 N=1,NDX1
000218      VOLN=ABED(N)*DX*VOIDF(N)
000219      W02V=WN2V+28./359.*492./(70.+460.)/760.*PN2*VOLN
000220      W02L=W02V+32./359.*492./(70.+460.)/760.*P02*VOLN
000221      600 CONTINUE
000222      WN2L=WN2L+WN2V
000223      W02L=W02L+W02V
000224      RN2L=WN2L/CYCLE/2.0
000225      R02L=W02L/CYCLE/2.
000226      WRITE(6,505) RN2L,R02L
000227      505 FORMAT(////' ESTIMATED CABIN GAS LOSSES'//
000228      1' NITROGEN LOSS (LB/HR) 'F8.4/
000229      2' OXYGEN LOSS (LB/HR) 'F8.4)
000230      GO TO NPRSBR
000231      END

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@ ELT DESORB, 1, 710719, 62340 , 1

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000001      SUBROUTINE DESORB
000002      C
000003      COMMON/AD/ TG(20),PH20I,TGI,PA,PK(2,20),PC021,TS(20)
000004      1,TC(20),TX(20),TS1(20),TS2(20),TX1(20),TX2(20),TC1(20),
000005      2TC2(20),W(4,20),PT(20),GMR,GMW,GVIS,PN2,P02,
000006      3 ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),
000007      4AVX(20),RHOC(20),RHOS(20),RHOS(20),RHOC(20),RHGX(20),
000008      5CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),
000009      6POUT(10),TIMET(10),WTACMS,WTSG,PUMP(10),VPUMP(10),CPP(20),
000010      7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,1DSORB(20),
000011      8 HXG(20),HXS(20),HXC(20),HSG(20),
000012      9SK(20),TKX(20),DH(20),DIF(20),GK(20),UC(20),T268,TOTCO2,TOTH20,
000013      1SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX,
000014      1 TOTKWH,HTR1(20),WC,TOTHTC,WCC,PC02A,VC02A,SABC02,TC02A,
000015      1RS1(20,9), A(20),F(20),C(20),VS(20),DVS(20),DVS1(20),RS(20),
000016      1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),
000017      2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),
000018      3FR(2,20), P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3
000019      4(20,4), C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20),
000020      5 WM(2),TIME,CYCLE,DTO,DTMAX,WI,TI,PC02C,
000021      6VOLCAB,RC02C,
000022      7NCYCLT,NPRINT,NCYCLE,NDCON,NTEMP,NSTART,NPR,DT,DTT(4),SARCOS
000023      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,
000024      1 CP1,CP2,X, C1P,C2P,C3P,D1P
000025      DIMENSION AS(20), PD(20)
000026      DIMENSION P4(20),VIST(2)
000027      DOUBLE PRECISION G,DPKOTS,DPKDWK,PD
000028      EQUIVALENCE (ASX,AXS),(AGX,AXG),(ASG,AGS),(HXS,HSX),(HXG,HGX),(HSG
000029      1,HGS)
000030      EQUIVALENCE (PS,P4)
000031      DIMENSION SPT(10), PET(10)
000032      EQUIVALENCE (SPT,VPUMP),(PET,PUMP)
000033      DATA VIST/0.014, 0.009/
000034      DATA RGAS/554./
000035      C
000036      IF(TIME.LE.1.E-5)PF13=3.
000037      NDR=NDR4-1
000038      DO 21 N=1,NDX1
000039      J=2
000040      P4(N)=PT(N)
000041      AS(N)=4.*3.1416*RS(N)**2
000042      I=IFN(N,NDXM)
000043      IF( I .EQ. 2) J=1
000044      VIS= X(N)*VIST(I)*(1,-X(N))*VIST(J)
000045      F(N)=2.494E-4*PT(N)**0.795*(VIS/0.0174)
000046      DO 20 NR=1,NDR4
000047      I=N
000048      C1(NR,N)=-CR2(I,NR)
000049      C2(NR,N)=CR1(I,NR)/DT+CR2(I,NR)+CR3(I,NR)
000050      20 C3(NR,N)=-CR3(I,NR)
000051      C
000052      C
000053      B(1,N)=C3(1,N)/C2(1,N)
000054      DO 21 J=2,NDR
000055      21 B(J,N)=C3(J,N)/(C2(J,N)-C1(J,N)*B(J-1,N))
000056      NDX=NDX1-1
000057      C TO TEMPORARILY STORE SURFACE LOADING
000058      DO 50 N=1,NDX1

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000059      50 WS(N)=W(NDR4,N)
000060
000061      C TO CALCULATE CS1,CS2,DS FOR SORBENT HEAT BALANCE EQUATION
000062      IF (NTEMP .EQ. 0 ) GO TO 111
000063      DO 12 N=1,NDX1
000064      I=IFN(N,NDXM)
000065      CS2(N)=DT/CPS(N)/RHOSB(N)*ASG(N)*GK(N)*WM(I)*DH(N)
000066      CS1(N) = CS2(N)*X(N)
000067      IF (N.EQ.1) GO TO 13
000068      IF (N.EQ.NDX1) GO TO 14
000069      S1=SK(N)/DX**2*(TS(N-1)-2.*TS(N)+TS(N+1))
000070      GO TO 15
000071      13 S1=SK(1)/DX**2*(TS(2)-TS(1))
000072      GO TO 15
000073      14 S1=SK(NDX1)/DX**2*(TS(NDX)-TS(NDX1))
000074      15 DS(N)=DT/CPS(N)/RHOSB(N)*(S1+ASG(N)*HSG(N)*(TG(N)-0.5*TS2(N))+1
000075      1ASX(N)*HXS(N)*(TX(N)-0.5*TS2(N)))
000076      RATIO = (DT+DTO)/DT
000077      T=(DT+DTO)/CPS(N)/RHOSB(N)
000078      T1=0.5*T*(ASG(N)*HSG(N)+ASX(N)*HXS(N))
000079      CS1(N)=RATIO*CS1(N)/(1.+T1)
000080      CS2(N)=RATIO*CS2(N)/(1.+T1)
000081      DS(N)=RATIO*DS(N)
000082      DS(N)=(DS(N)-T1*TS2(N))/(1.+T1)
000083      12 CONTINUE
000084      GO TO 110
000085      111 DO 112 N=1,NDX1
000086      CS1(N)=0,
000087      CS2(N)=0,
000088      DS(N)=0,
000089      TS(N)=T268
000090      TC(N)=T268
000091      TX(N)=T268
000092      TG(N)=T268
000093      112 CONTINUE
000094      110 CONTINUE
000095      C TO CALCULATE TOTAL PRESSURE
000096
000097      C
000098      DO 24 N=1,NDX1
000099      I=IFN(N,NDXM)
000100      C TO CALCULATE P1,P2,P3
000101      WSURF=W(NDR4,N)
000102      CALL EQPWT(I,IDSORB(N),1,PSURF,WSURF,TS2(N))
000103      CALL EQPWT(I,IDSORB(N),1,PS1,    WSURF,(TS2(N)+0.02))
000104      DPKDTS=(PS1-PSURF)/0.02
000105      CALL EQPWT(I,IDSORB(N),1,PS2,(WSURF+1.E-5),TS2(N))
000106      DPKDWK=(PS2-PSURF)/1.E-5
000107      G=1.+CS2(N)*DPKDTS
000108      P1(N)=(PSURF               +DS(N)*DPKDTS)/G
000109      P2(N)=DPKDWK/G
000110      P3(N)=CS1(N)/G*DPKDTS
000111      C
000112      C2(NDR4,N)=CR1(N,NDR4)/DT+CR2(N,NDR4)+WM(I)*GK(N)*P2(N)*AS(N)
000113      C3(NDR4,N)=0.0
000114      DO 23 NR=1,NDR4
000115      23 D1(NR,N)=CR1(N,NR)/DT*W(NR,N)
000116      D1(NDR4,N)=D1(NDR4,N)-WM(I)*GK(N)*(P1(N)-P2(N)*W(NDR4,N))*AS(N)
000117      D2(N)=AS(N)*WM(I)*GK(N)*(X(N)   -P3(N))
000118      D2(N)=D2(N)/(C2(NDR4,N)-C1(NDR4,N)*B(NDR4-1,N))

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000119      Q(1,N)=D1(1,N)/C2(1,N)
000120      DO 24 J=2,NDR4
000121      24 Q(J,N)=(D1(J,N)-C1(J,N)*Q(J-1,N))/(C2(J,N)-C1(J,N)*B(J-1,N))
000122
000123      C      COEFFICIENTS FOR P-EQUATION
000124      DO 25 N=2,NDX
000125      25 PC2(N) = PT(N)/(VOIDF(N)*C(N)*ABED(N))*(VOIDF(N+1)*C(N+1)*ABED(N+1)
000126      1)/F(N+1) - VOIDF(N-1)*C(N-1)*ABED(N-1)/F(N-1)/(2.*DX)
000127      N=1
000128      PC2(N) = PT(N)/(VOIDF(N)*C(N)*ABED(N))*(VOIDF(N+1)*C(N+1)*ABED(N+1)
000129      1)/F(N+1) - VOIDF(N)*C(N)*ABED(N)/F(N))/(1.*DX)
000130      N= NDX1
000131      PC2(N) = PT(N)/(VOIDF(N)*C(N)*ABED(N))*(VOIDF(N-1)*C(N-1)*ABED(N-1)
000132      1)/F(N-1) - VOIDF(N-1)*C(N-1)*ABED(N-1)/F(N-1))/(1.*DX)
000133      DO 26 N=1,NDX1
000134      PC1(N)=PT(N)/F(N)
000135      26 PC3(N)=PT(N)/C(N)/VOIDF(N)*ASG(N)*GK(N)
000136
000137      C      DO 27 N=1,NDX1
000138      CP1(N)=PC3(N)*(P1(N)+P2(N)*(Q(NDR4,N)-W(NDR4,N)))
000139      CP2(N)=PC3(N)*(P2(N)+P2(N)+P3(N))           -X(N))
000140      C1P(N)=-PC1(N)/DX/DX+PC2(N)/2./DX
000141      C2P(N)=1./DT+2.*PC1(N)/DX/DX-CP2(N)
000142      C3P(N)=-PC1(N)/DX/DX-PC2(N)/2./DX
000143      27 D1P(N)=PT(N)/DT+CP1(N)
000144
000145      C      BOUNDARY CONDITION FOR P-EQUATION
000146
000147      C2P(1)=C2P(1)*C1P(1)
000148      C1P(1)=0.
000149      GO TO (55,56,58,58), NBCOUT
000150
000151      58 CONTINUE P PUMP CHARACTERISTIC GIVEN
000152      POP1=PC02A*51.7/PT(NDX1)
000153      CALL LAGIN2( 58,PUMP,10.2,POP1,VPUMP1,VPUMP)
000154      VPUMP1=VPUMP1*(TG(NDX1)+460.)/(TC02A+460.)
000155      IF(VPUMP1 .LT. 0.0) VPUMP1=0.00
000156      CEXIT=VPUMP1*60./(ABED(NDX1)*VOIDF(NDX1))/PT(NDX1)
000157      GO TO 59
000158
000159      55 CONTINUE
000160      EMW=X(NDX1)*WM(2)+(1.-X(NDX1))*WM(1)
000161      EVIS=X(NDX1)*VIST(2)+(1.-X(NDX1))*VIST(1)
000162      EVIS=EVIS*0.01
000163      SQTM= SGRT( (TG(NDX1)+460.)/1.8/EMW)
000164      DIA=6.0
000165      TOTL=127.
000166      PTAVG=0.5*(PT(NDX1)+PF13)
000167      EV=3.269E-2*PTAVG*          DIA**4/TOTL/EVIS+
13.81*DIA**3/TOTL*(SQTM*0.147*PTAVG*          DIA/EVIS)
000168      2/(SOTM*0.181*PTAVG*          DIA/EVIS)
000169      EV=EV*3600./28.316
000170      EV1=EV
000171      N1=1
000172
000173      91 CONTINUE
000174      QF=(PT(NDX1)-PF13)*EV
000175      CALL LAGIN2(58,PET,10.2,PF13,SP,SPT)
000176      DGF=QF-SP*PF13
000177      CALL NEWTO2(N1,NGO,PF13,DGF,PF130,DGF0,1.E-3,PT(NDX1),0.0111)
000178      GO TO (91,92), NGO
000179      92 CONTINUE

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000179      EV=SP*EV/(SP+EV)
000180      C2P(NDX1)=C2P(NDX1)+C3P(NDX1)*(1.-EV*F(NDX1)*DX/VOIDF(NDX1)/ABED
000181      1(NDX1)/PT(NDX1))
000182      C3P(NDX1)=0.000
000183      GO TO 57
000184
000185      C 59 C2P(NDX1) = C2P(NDX1)+C3P(NDX1)*(1.-DX*F(NDX1)*CEXIT)
000186      C3P(NDX1)=0.0
000187      GO TO 57
000188      56 CONTINUE
000189      C PRESSURES ARE SET
000190
000191      DO 561 K= 1, 3
000192      IF(NPSET(K) .EQ. 0) GO TO 561
000193      NP=NPSET(K)
000194      C1P(NP)=0.0
000195      C2P(NP)=1.0
000196      C3P(NP)=0.0
000197      CALL LACIN2(10,TIMET,10,2,TIME,D1PNP ,POUT)
000198      D1P(NP)=D1PNP
000199      561 CONTINUE
000200      57 CONTINUE
000201      CALL FDEQID(C1P,C2P,C3P,D1P,PD,NDX1)
000202      DO 34 N=1,NDX1,
000203      IF(PD(N) .LE. 0.) PD(N) = 1.E-3
000204      34 PT(N)=PD(N)
000205
000206      C TO CALCULATE SORBENT LOADING
000207
000208      DO 30 N=1,NDX1
000209      W(NDR4,N)=Q(NDR4,N)+D2(N)*PT(N)
000210      DO 30 J=2,NDR4
000211      L=NDR4+1-J
000212      30 W(L,N)=Q(L,N)-B(L,N)*W(L+1,N)
000213
000214      C TO CALCULATE STREAM COMPOSITION
000215
000216      FR(1,1) = 0.0
000217      FR(2,1)=0,
000218      FR2=0.0
000219      DO 31 N=1,NDX1
000220      I=IFN(N,NDXM)
000221      TEMP =C(N)*VOIDF(N)
000222      1/P4(N)*ABED(N) *DX*(CP1(N)+CP2(N)*PT(N))
000223      IF(I.EQ.1)J=2
000224      IF(I.EQ.2)J=1
000225      IF(N . EQ. 1) GO TO 200
000226      FR(J,N)=FR(J,N-1)
000227      FR(I,N)=TEMP+FR(I,N-1)
000228      IF( NDXM .EQ. 0) GO TO 202
000229      IF ( I .EQ. 1) GO TO 202
000230      IF(NPSET(2)..NE. 0) GO TO 202
000231      GO TO 201
000232      200 FR(I,1) = TEMP
000233      202 X(N) = 1.0
000234      GO TO 31
000235      201 CONTINUE
000236      CT=ABED(N)*DX*ASG(N)*GK(N)
000237      FRT= FR(1,N)+FR(2,N)+1.E-10
000238      PSURF = P1(N)+P2(N)*(W(NDR4,N)-WS(N))+P3(N)*PT(N)

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000239      X(N)=((FR(2,N-1)+CT*PSURF)          )/FRT/
000240      1 *(1.+CT*PT(N)/FRT)
000241      IF(X(N) .LT. 0.0) X(N)=0.0
000242      IF(X(N) .GT. 1.0) X(N)=1.0
000243 31 CONTINUE
000244      DO 33 N=1,NDX1
000245      C(N) = (PT(N)/RGAS/(TG(N)+460)+C(N))/2.0
000246      I = IFN (N,NDXM)
000247      IF (I.EQ.1) J=2
000248      IF (I.EQ.2) J=1
000249      RHOG(N)=C(N)*(X(N)*WM(I)+(1.-X(N))*WM(J))
000250      UG(N)=(FR
000251      1 *(1,N)*WM(1)+FR(2,N)*WM(2))/RHOG(N)/ABED(N)/VOIDF(N)
000252
000253      33 CONTINUE
000254      IF( NTEMP .EQ. 0) RETURN
000255      C      TO CALCULATE SORBENT TEMPERATURES
000256      C
000257      CALL TSCRB
000258      D9=DT
000259      CALL TGLCOL(TC,NDX1,UC,RHOC,CPC,CX,AXC,HXC,T268,TX,DX,D9,
000260      1AVC, NOG ,DT0,TS1,TS2,TX1,TX2,TC1,TC2)
000261      CALL HXCORE
000262      CALL GAST(DX,RHOG,CPG,UG,TS,TX,NDX1,ASG,HSG,AXG,HXG,TG,VOIDF)
000263 100 FORMAT(8G12.3)
000264      DESRAT=FR(1,NDX1)
000265      IF(NBCOUT .EQ. 3) GO TO 101
000266      IF(NBCOUT .EQ. 4) GO TO 1018
000267      RETURN
000268 101 CONTINUE
000269      DPC02A=(DESRAT-SABC02/44.)*DT*RGAS*(TC02A+460.0)/VC02A/51.7
000270      PC02A=PC02A+DPC02A
000271      RETURN
000272 1018 CONTINUE
000273      DVC02A =(DESRAT -SABC02/44.0)*DT*RGAS*(TC02A+460.0)/PC02A/51.7
000274      VC02A=VC02A+DVC02A
000275      RETURN
000276      END

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@ ELT EQPWT,1,710712, 56799 , 1

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000001      SUBROUTINE EQPWT(ID,IDSORB,KPW,P,W,T)
000002      C   KPW=1 = W,T TO FIND P
000003      C   KPW=2 = P,T TO FIND W
000004      C   PKEQ=EQUILIBRIUM PRESSURE IN MM HG
000005      C   W=LOADING IN LB ADSORBATE PER LB ADSORBENT
000006      C   T=TEMP IN DEG F
000007      C
000008      DIMENSION TTAB(10,25), WTAB(15,10,25), PTAB(15,10,25), NT(25)
000009      DIMENSION IDSMTX(5,5)
000010      C   NT(1) DATA FOR CO2 ON MOL SIEVE 5A
000011      C   NT(2) DATA FOR H2O ON MOL SIEVE 5A
000012      C   NT(3) DATA FOR H2O ON SILICA GEL
000013      C   NT(4) DATA FOR CO2 ON MOL SIEVE 13X
000014      C   NT(5) DATA FOR H2O ON MOL SIEVE 13X
000015      DATA IDSMTX/1.0,4.0,0.0,2.3,5, 0.0, 6.0,8.0,0.7,0.9,0.0,0.0,0.0,0.0/
000016      DATA JACK/0/
000017      DATA NT/25*0.0/
000018      C
000019      DATA NT(1)/6/
000020      DATA (TTAB(J,1),J=1,6)/392.,212.,122.,77.,51.,32./
000021      DATA (WTAB(I,1,1),I=1,15)/.001,.0018,.0021,.0025,.003,.0037,.004,
000022      .0045,.005,.0055,.0063,.007,.008,.0088,.0092/
000023      DATA (PTAB(I,1,1),I=1,15)/1.0,1.5,2.0,2.5,3.0,4.0,5.0,7.0,8.0,10.,
000024      115.,20.,30.,40.,50./
000025      DATA (WTAB(I,2,1),I=1,15)/.002,.0028,.004,.0047,.0052,.006,.007,
000026      1.009,.01,.012,.015,.019,.025,.03,.034/
000027      DATA (PTAB(I,2,1),I=1,15)/1.0,1.5,2.0,2.5,3.0,4.0,5.0,7.0,8.0,10.,
000028      115.,20.,30.,40.,50./
000029      DATA (WTAB(I,3,1),I=1,15)/.00009,.0018,.0025,.0027,.0043,
000030      10.0065.0.0145.0.0178.0.0265.0.0325.0.04.0.0485.0.057.0.07/
000031      DATA(WTAB(I,5,1),I=1,15)/.0002,0.005,0.008,0.0122,0.018,0.0255,
000032      10.0324.0.04,0.05,0.07,0.08,0.09,0.1,0.11,0.1177/
000033      DATA(WTAB(I,6,1),I=1,15)/.0016,0.0035,0.0073,0.01,0.015,0.02,
000034      10.0277,0.04,0.05,0.06,0.077,0.09,0.1,0.11,0.12/
000035      DATA (PTAB(I,3,1),I=1,15)/.05,.1,2,.3,.7,1,.1,9,3,.4,.7,,
000036      110.,14.5,20.,26.,40./
000037      DATA (WTAB(I,4,1),I=1,15)/.0009,.0025,.0033,.006,.0093,.013,
000038      10.0174,.027,.0347,.041,.05,.06,.08,.0955,.103/
000039      DATA (PTAB(I,4,1),I=1,15)/.03,.06,.1,.2,.4,.7,1,.2,,
000040      13,.4,.5,.6,.7,.7,13,.20,.26.5/
000041      DATA (PTAB(I,5,1),I=1,15)/.02,.05,.1,.2,.4,.7,1,.1.5,
000042      12.17,3.9,5.7,10,.15,.20./
000043      DATA (PTAB(I,6,1),I=1,15)/.01,.03,.06,.1,.2,.3,.5,.88,
000044      11.32,1.8,3,.4,65.6,6,9.5,15./
000045      C
000046      DATA NT(2)/6/
000047      DATA (TTAB(J,2),J=1,6)/392.,212.,167.,122.,77.,32./
000048      DATA (WTAB(I,1,2),I=1,15)/.004,.007,.01,.012,.015,.018,.02,.023,
000049      1.028,.038,.05,.071,.076,.081,.09/
000050      DATA (PTAB(I,1,2),I=1,15)/.01,.02,.05,.1,.2,.5,1,.2,.5,.10,.20.,
000051      150.,60.,75.,100./
000052      DATA (WTAB(I,2,2),I=1,15)/.02,.024,.026,.030,.036,.045,.051,.058,
000053      1.074,.091,.11,.135,.15,.16,.175/
000054      DATA (PTAB(I,2,2),I=1,15)/.01,.02,.03,.05,.1,.2,.3,.5,1.0,2.0,
000055      14.0,.10,.20,.40,.100/
000056      DATA (WTAB(I,3,2),I=1,15)/.027,.035,.038,.045,.057,.071,.08,.092,
000057      1.11,.125,.135,.145,.16,.18,.19/
000058      DATA (PTAB(I,3,2),I=1,15)/.01,.02,.03,.05,.1,.2,.3,.5,1,.2,.3,.4,,

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000059      110.,60.,120./
000060      DATA (WTAB(I,4,2),I=1,15)/.045,.058,.065,.078,.097,.115,.125,.135,
000061      1.145,.160,.165,.175,.180,.185,.188/
000062      DATA (PTAB(I,4,2),I=1,15)/.01,.02,.03,.05,.1,.2,.3,.5,.1,.2,.3,.10,
000063      1.20,.60,.120./
000064      DATA (WTAB(I,5,2),I=1,15)/.083,.103,.115,.12,.14,.155,.159,.163,
000065      1.175,.18,.181,.182,.183,.184,.185/
000066      DATA (PTAB(I,5,2),I=1,15)/.01,.02,.03,.04,.1,.2,.3,.5,.1,.2,.4,.7.,
000067      115,.40,.100./
000068      DATA (WTAB(I,6,2),I=1,15)/.135,.15,.155,.16,.167,.169,.173,.178,.18
000069      10,.181,.183,.184,.185,.186,.187/
000070      DATA (PTAB(I,6,2),I=1,15)/.01,.02,.03,.04,.07,.10,.20,.50,1.5,3.0,
000071      17.0,15.0,30.0,70.0,100.0/
000072      C
000073      DATA NT(3)/5/
000074      DATA (TTAB(J,3),J=1,5)/160.,100.,60.,40.,10./
000075      DATA (WTAB(I,1,3),I=1,15)/.0018,.0026,.0031,.0057,.008,.01,.03,
000076      1.06,.10,.14,.20,.32,.45,.49,.50/
000077      DATA (PTAB(I,1,3),I=1,15)/.01,.05,.1,.4,1.0,1.95,9.42,23.6,44.8,
000078      167.2,101.8,200.,400.,700.,1000./
000079      DATA (WTAB(I,2,3),I=1,15)/.00305,.005,.0069,.009,.02,.05,.07,.11,
000080      1.17,.215,.32,.42,.50,.58,.59/
000081      DATA (PTAB(I,2,3),I=1,15)/.01,.05,.10,.2,.87,3.20,5.04,9.06,15.6,
000082      120.,30.,50.,100.,300.,700./
000083      DATA (WTAB(I,3,3),I=1,15)/.005,.008,.01,.02,.04,.05,.06,.10,.19,
000084      1.27,.405,.50,.55,.60,.64/
000085      DATA (PTAB(I,3,3),I=1,15)/.01,.03,.07,.206,.574,.79,1.02,2.04,4.7,
000086      17.23,15.,30.,50.,100.,300./
000087      DATA (WTAB(I,4,3),I=1,15)/.008,.0092,.01,.02,.03,.05,.07,.11,.27,
000088      1.40,.42,.48,.57,.67,.75/
000089      DATA (PTAB(I,4,3),I=1,15)/.01,.02,.03,.092,.17,.36,0.58,1.08,3.45,
000090      16.0,8.0,10.0,20.0,70.0,200.0/
000091      DATA (WTAB(I,5,3),I=1,15)/.014,.018,.022,.05,.08,.205,.28,.35,.42,
000092      1.50,.60,.70,.77,.80,.82/
000093      DATA (PTAB(I,5,3),I=1,15)/.01,.02,.03,.10,.20,.70,1.0,1.5,2.0,3.0,
000094      15.0,10.0,20.0,40.0,100.0/
000095      C
000096      DATA NT(4)/3/
000097      DATA (TTAB(J,4),J=1,3)/122.,77.,32./
000098      DATA (WTAB(I,1,4),I=1,15)/.00355,.0036,.00365,.0037,.0038,.0040,
000099      1.0045,.005,.0059,.0077,.011,.016,.020,.026,.037/
000100      DATA (PTAB(I,1,4),I=1,15)/.02,.03,.04,.05,.07,.10,.20,.30,.50,1.0,
000101      12.0,4.0,6.0,10.0,20.0/
000102      DATA (WTAB(I,2,4),I=1,15)/.0098,.01,.0105,.0115,.0124,.0133,.0150,
000103      1.0165,.018,.021,.033,.0415,.0475,.055,.064/
000104      DATA (PTAB(I,2,4),I=1,15)/.025,.05,0.1,0.2,0.3,0,4,0.6,0.8,1.0,1.5
000105      1.4,0,7,0,10,0,15,0,25,0/
000106      DATA (WTAB(I,3,4),I=1,15)/.018,.0187,.0191,.02,.0222,.0248,.0282,
000107      1.031,.033,.0355,.04,.05,.068,.078,.093/
000108      DATA (PTAB(I,3,4),I=1,15)/.002,.01,.02,.04,.10,.20,.40,.60,.80,1.,
000109      11.5,3.0,6.0,10.0,20.0/
000110      C
000111      DATA NT(5)/6/
000112      DATA (TTAB(J,5),J=1,6)/400.,300.,200.,122.,77.,35./
000113      DATA (WTAB(I,1,5),I=1,15)/.0001,.0002,.0005,.001,.002,.003,
000114      1.005,.01,.016,.022,.03,.041,.05,.06,.07/
000115      DATA (PTAB(I,1,5),I=1,15)/.001,.002,.005,.01,.02,.05,.1,.2,.5,
000116      11,.2,.5,.10,.20,.50/
000117      DATA (WTAB(I,2,5),I=1,15)/.001,.002,.003,.004,.009,.012,.018,
000118      1.025,.038,.048,.06,.078,.09,.102,.118/

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000119 DATA (PTAB(I,2,5),I=1,15)/.001,.002,.005,.01,.02,.05,.1,.2,.5,
 000120 11.,2.,5.,10.,20.,50./
 000121 DATA (WTAB(I,3,5),I=1,15)/.007,.01,.015,.02,.026,.036,.046,.056,
 1.075,.09,.104,.124,.14,.153,.17/
 000122 DATA (PTAB(I,3,5),I=1,15)/.001,.002,.005,.01,.02,.05,.1,.2,.5,
 11.,2.,5.,10.,20.,50./
 000123 DATA (WTAB(I,4,5),I=1,15)/.049,.052,.054,.059,.067,.083,.096,
 1.116,.132,.152,.164,.180,.196,.208,.225/
 000124 DATA (PTAB(I,4,5),I=1,15)/.001,.003,.005,.01,.02,.05,.09,.2,
 1.35,.72,1.013,2.23,4.65,8.5,20./
 000125 DATA (WTAB(I,5,5),I=1,15)/.068,.072,.078,.090,.105,.124,.14,
 1.156,.165,.182,.196,.209,.224,.24,.256/
 000126 DATA (PTAB(I,5,5),I=1,15)/.001,.003,.005,.01,.02,.05,.1,.2,.3,
 1.6,1.1,2.0,4.0,9.0,19./
 000127 DATA (WTAB(I,6,5),I=1,15)/.108,.112,.13,.144,.158,.172,
 1.186,.198,.213,.224,.236,.252,.268,.28,.30/
 000128 DATA (PTAB(I,6,5),I=1,15)/.001,.002,.005,.01,.02,.04,.08,.15,.3,
 1.5,.85,1.7,3.5,6.2,20./
 C
 000129 DATA NT(6)/3/
 000130 DATA (TTAB(J,6), J=1,3)/120., 68., 32./
 000131 DATA(PTAB(I,1,6),I=1,15) / 15., 20., 30., 40., 60., 80., 100., 125., 150.
 1,200., 250., 350., 450., 600., 750./
 000132 DATA(PTAB(I,2,6),I=1,15) / 15., 20., 30., 40., 60., 80., 100., 125., 150.
 1,200., 250., 350., 450., 600., 750./
 000133 DATA(PTAB(I,3,6),I=1,15) / 15., 20., 30., 40., 60., 80., 100., 125., 150.
 1,200., 250., 350., 450., 600., 750./
 000134 DATA (WTAB(I,1,6),I=1,15)/.0005,.0007, .0009,.00116,,00137,
 1.00155,.00178,.00205,.00250,.0031,.00435,.00565,.0073,.0087/
 000135 DATA (WTAB(I,2,6),I=1,15)/.0007,.00078,.00102,.00126,.00173,
 1.00207,.00205,.0030,.00348,.0044,.0052,.0068,.0083,.0103,.0122/
 000136 DATA (WTAB(I,3,6),I=1,15)/
 1.0012,.0014,.0019,.0023,.0030,.0037,.00435,.0052,.00602,
 2.0075,.0087,.0138,.0137,.0167,.0197/
 000137 DATA NT(7)/2/
 000138 DATA (TTAB(J,7),J=1,2)/70., 32./
 000139 DATA (PTAB(I,1, 7),I=1,15)/
 110.,15.,20.,30.,40.,55.,75.,100.,125.,150.,200.,300.,400.,550.,750
 2./
 000140 DATA (PTAB(I,2, 7),I=1,15)/
 110.,15.,20.,30.,40.,55.,75.,100.,125.,150.,200.,300.,400.,550.,750
 2./
 000141 DATA (WTAB(I,1,7),I=1,15)/
 1.0002,.00025,.0003,.00043,.0005,.00065,.00082,.00105,.00125,.00146
 2,.00186,.00264,.0034,.0044,.00555/
 000142 DATA (WTAB(I,2,7),I=1,15)/
 1.0002,.00025,.0003,.00044,.00056,.00073,.00096,.00122,.00148,
 2.00173,.00224,.00337,.00447,.00585,.0074/
 000143 DATA NT(8)/3/
 000144 DATA(TTAB(J,8),J=1,3)/120.,72.,32./
 000145 DATA (PTAB(I,1, 8),I=1,15)/
 110.,15.,20.,30.,40.,55.,75.,100.,125.,150.,200.,300.,400.,550.,750
 2./
 000146 DATA (PTAB(I,2, 8),I=1,15)/
 110.,15.,20.,30.,40.,55.,75.,100.,125.,150.,200.,300.,400.,550.,750
 2./
 000147 DATA (PTAB(I,3, 8),I=1,15)/
 110.,15.,20.,30.,40.,55.,75.,100.,125.,150.,200.,300.,400.,550.,750
 2./
 000148 DATA (WTAB(I,1,8),I=1,15)/



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000179      1.0001,.0002,.0003,.0004,.0005,.0006,.00075,.0008,.001,.00115,
000180      2.0014,.002,.00255,.0035,.0047/
000181      DATA (WTAB(I,2,8),I=1,15)/
000182      1.00035,.0004,.00045,.0005,.0006,.0009,.0012,.00155,.0018,.0022,
000183      2.0028,.004,.0052,.0066,.0084/
000184      DATA (WTAB(I,3,8),I=1,15)/
000185      1.00065,.0007,.00085,.001,.0012,.0014,.0017,.0024,
000186      2.0032,.0038,.0050,.0069,.0085,.0108,.0144/
000187      DATA NT(9)/3/
000188      DATA (TTAB(J,9),J=1,3)/120.,72.,32./
000189      DATA (PTAB(I,1, 9),I=1,15)/
000190      110..15..20..30.,40..55..75..100..125..150..200..300..400..550..750
000191      2./
000192      DATA (PTAB(I,2, 9),I=1,15)/
000193      110..15..20..30.,40..55..75..100..125..150..200..300..400..550..750
000194      2./
000195      DATA (PTAB(I,3, 9),I=1,15)/
000196      110..15..20..30.,40..55..75..100..125..150..200..300..400..550..750
000197      2./
000198      DATA (WTAB(I,1,9),I=1,15)/
000199      1.0001,.00013,.00017,.0002,.00025,.0003,.00037,.00048,.00058,
000200      2.00067,.00087,.00122,.00163,.00221,.00291/
000201      DATA (WTAB(I,2,9),I=1,15)/
000202      1.0002,.00023,.00026,.00036,.00045,.00058,.0007,.00085,
000203      2.00092,.00111,.00136,.0019,.0024,.00312,.00396/
000204      DATA (WTAB(I,3,9),I=1,15)/
000205      1.00025,.00034,.00042,.00055,.00067,.00082,.001,.00122,
000206      2.00144,.00163,.00199,.00264,.00328,.0043,.00578/
000207      C
000208      IF (W .LE. 0. ) W= 1.E-20
000209      IF(JACK .GT. 0) GO TO 102
000210      DO 105 K=1,25
000211      IF (NT(K) .EQ. 0) GO TO 90
000212      NTI=NT(K)
000213      DO 101 J=1,NTI
000214      TTAB(J,K)=1./(TTAB(J,K)+460.)
000215      DO 101 I=1,15
000216      WTAB(I,J,K)= ALOG(WTAB(I,J,K))
000217      PTAB(I,J,K)= ALOG(PTAB(I,J,K))
000218      101 CONTINUE
000219      90 CONTINUE
000220      105 CONTINUE
000221      102 CONTINUE
000222      IS=IDSMTX(IDSORB, ID)
000223      IF(IS.EQ.0) GO TO 999
000224      JACK = JACK + 1
000225      RT=1./(T+460.)
000226      GO TO (201,202), KPW
000227      201 WL=ALOG(W)
000228      N=NT(IS)
000229      PKEQ1=XYZMAP(1,WTAB(1,1,IS), PTAB(1,1,IS),15,TTAB(1,IS),N ,2,2,WL,
000230      ,1RT,ANS)
000231      P   =EXP(PKEQ1)
000232      IF (PKEQ .LT. 0.0) PKEQ=0.0
000233      RETURN
000234      202 PL=ALOG(P)
000235      N=NT(IS)
000236      W01=XYZMAP(1,PTAB(1,1,IS),WTAB(1,1,IS),15,TTAB(1,IS),N,2,2,PL,RT,
000237      ,1ANS)
000238      W=EXP(W01)

000239      RETURN
000240      999 WRITE(6,998) IDSORB, ID
000241      998 FORMAT(////' EQUILIBRIUM DATA UNAVAILABLE FOR'// IDSORB ='14/''
000242      1 ID =' 14)
000243      CALL EXIT
000244      END

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@ ELT FCOAD,1,710712, 56800 , 1

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000001      FUNCTION FCOAD(IDSORB,H20)
000002      C
000003      C
000004      DIMENSION H20T(12), FCOADT(12,5)
000005      DATA H2CT/ .00, .01, .02, .03, .04, .05, .06, .07, .08, .10,
000006      1.12, .60/
000007      DATA (FCOADT(I,1),I=1,12)/1.,.98,.88,.72,.575, .436, .313, .22,
000008      1.155, .086, .055, .0/
000009      DATA(FCCADT(1,3),I=1,12)/1., .794, .63, .503, .415, .35, .298,
000010      1.252, .214, .148, .085, .0/
000011      CALL LAGIN2(666, H20T      ,12,2,H20,FCOAD,FCOADT(1,IDSORB))
000012      RETURN
000013      END

```

@ ELT FDEQID,1,710514, 38495 , 1

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000001      SUBROUTINE FDEQID(C1,C2,C3,D,VAR,NN)
000002      DIMENSION C1(1),C2(1),C3(1),D(1),VAR(1),B(41),Q(41)
000003      DOUBLE PRECISION C1,C2,C3,D,VAR,B,Q
000004      NN1=NN-1
000005      B(1)=C3(1)/C2(1)
000006      DO 41 J=2,NN1
000007      41 B(J)=C3(J)/(C2(J)-C1(J)*B(J-1))
000008      Q(1)=D(1)/C2(1)
000009      DO 42 J=2,NN
000010      42 Q(J)=(D(J)-C1(J)*Q(J-1))/(C2(J)-C1(J)*B(J-1))
000011      VAR(NN)=Q(NN)
000012      DO 43 J=2,NN
000013      43 L=NN+1-J
000014      43 VAR(L)=Q(L)-B(L)*VAR(L+1)
000015      RETURN
000016      END

```

@ ELT FDEQIM,1,710514, 38492 , 1

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000001      SUBROUTINE FDEQIM(C1,C2,C3,D,VAR,NN)
000002      DIMENSION C1(1),C2(1),C3(1),D(1),VAR(1),B(41),Q(41)
000003      NN1=NN-1
000004      B(1)=C3(1)/C2(1)
000005      DO 41 J=2,NN1
000006      41 B(J)=C3(J)/(C2(J)-C1(J)*B(J-1))
000007      Q(1)=D(1)/C2(1)
000008      DO 42 J=2,NN
000009      42 Q(J)=(D(J)-C1(J)*Q(J-1))/(C2(J)-C1(J)*B(J-1))
000010      VAR(NN)=Q(NN)
000011      DO 43 J=2,NN
000012      43 L=NN+1-J
000013      43 VAR(L)=Q(L)-B(L)*VAR(L+1)
000014      RETURN
000015      END

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@ ELT FLAP,1,710719, 62342 , 1

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000001      SUBROUTINE FLAP
000002      COMMON/AD/ TG(20),PH20I ,TGI ,PA ,          PK (2,20),PC021 ,TS (20)      *NEW
000003      1,TC (20),TX (20), TS1 (20),TS2 (20),TX1 (20),TX2 (20),TC1 (20),      *NEW
000004      2TC2 (20),W (4,20),PT (20),          GMR ,GMW,GVIS, PN2,P02,      *NEW
000005      3,ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),      *NEW
000006      4AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),      *NEW
000007      5CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),      *NEW
000008      6POUT(10),TIMET(10),WTACMS,WTSG ,PUMP(10),VPUMP(10),CPP(20),      *NEW
000009      7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20),      *NEW
000010      8,HXG(20),HXS(20),HXC(20),HSG(20),      *NEW
000011      9SK(20),TKX(20),DH(20),DIF(20),GK(20),UC(20),T268,TOTCO2,TOTH20,      *NEW
000012      1SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX;      *NEW
000013      1 TOTKWH,HTR1(20),WC,TOTHTC,WCC,PC02A,VC02A,SABC02, TC02A,      *NEW
000014      1RS1(20,9), A(20),F(20),C(20),VS(20),DVS(20),DVS1(20),RS(20),      *NEW
000015      1UG(20),PS(20),DS(20),CS(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),      *NEW
000016      2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),      *NEW
000017      3FR(2,20), P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3      *NEW
000018      4(20,4), C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20),      *NEW
000019      5 WM(2),TIME,CYCLE,DT0, DTMAX,WI,TI,PC02C,      *NEW
000020      6VOLCAB,RC02C,      *NEW
000021      7NCYCLT,NPRINT,NCYCLE,NDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SABCOS      *NEW
000022      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,      *NEW
000023      1 CP1,CP2,X, C1P,C2P,C3P,D1P,      *NEW
000024      DIMENSION DUMMY(20),DUMM1(20),IDUMMY(20)      *NEW-1
000025      NAMELIST /CHECK/
000026      1TG,PH20I,TGI,PA,PK,PC021,TS,TC,TX,TS1,TS2,TX1,TX2,TC1,TC2,W,PT,
000027      2GMR,GMW,ABED,AVC,ASG,ASX,AGX,AXC, AVX,RHOG,RHOSB,RHOS,RHOC,RHOX,CP
000028      3G, CPC,CPX,CPS,DX,POUT,TIMET,WTACMS,WTSG ,PUMP,VPUMP,NPSET,NDR4,
000029      4NDXMAC,NBCOUT,NDX1,NDXM,NOG,HXG,HXS,HXC,HSG,SK,TKX,DH,DIF,GK,UC,T2
000030      568, TOTCO2,TOTH20,SUMPTM,AVMSL1,AVSGL1,HTR,TMAX,A,F,C,VS,DVS,DVS1
000031      CALL FLIP(W,TG,TS,TX,TC,NDX1,NDR4,NOG,UC)
000032      CALL FLCP(ABED,AVC,ASG,ASX,AGX,NDX1)
000033      CALL FLOP(AXC,AVX,RHOG,RHOSB,RHOC,NDX1)
000034      CALL FLOP(RHOX,CPG,CPC,CPX,CPS,NDX1)
000035      CALL FLOP(HXG,HXS,HXC,HSG,DH,NDX1)
000036      CALL FLOP(DIF,GK,PT ,X ,HTR ,NDX1)
000037      CALL FLOP(TS1,DUMMY,DUMMY,DUMMY,DUMMY,NDX1)
000038      CALL FLOP(TS2,TX1,TX2,TC1,TC2,NDX1)
000039      NDX2=NDX1+1
000040      CALL FLOP(SK,TKX,DUMMY,DUMMY,DUMMY,NDX2)
000041      DO 61 K=1,2
000042      DO 62 N=1, NDX1
000043      DUMM1(N)=FR(K,N)
000044      62 DUMMY(N)=PK(K,N)
000045      DO 61 N=1,NDX1
000046      I=NDX1+1-N
000047      FR(K,1)=DUMM1(N)
000048      61 PK(K,1)=DUMMY(N)
000049      DO 63 N=1,NDX1
000050      63 IDUMMY(N)=IDSORB(N)
000051      DO 64 N=1,NDX1
000052      I=NDX1+1-N
000053      64 IDSORB(1)=IDUMMY(N)
000054      RETURN
000055      END

```

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* ELT FLIP,1,710514, 38498 , 1

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```
000001      SUBROUTINE FLIP(W,TG,TS,TX,TC,NX,NOG,UC).
000002      C   THIS SUBROUTINE INVERTS BED LOADINGS AND TEMPERATURES
000003      DIMENSION W( 4,20),TG(20),TS(20),TX(20),TC(20),UC(20)
000004      DIMENSION TW( 4,20),TTG(20),TTS(20),TTX(20),TTC(20),TUC(20)
000005      DO 5 I=1,NX
000006      CO 6 J=1,NR
000007      6 TW(J,I)=W(J,I)
000008      TTC(I)=TC(I)
000009      TTG(I)=TG(I)
000010      TTS(I)=TS(I)
000011      TTX(I)=TX(I)
000012      5 TUC(I)=UC(I)
000013      DO 10 N=1,NX
000014      I=NX+1-N
000015      DO 15 J=1,NR
000016      15 W(J,I)=TW(J,N)
000017      TG(I)=TTG(N)
000018      TS(I)=TTS(N)
000019      TX(I)=TTX(N)
000020      TC(I)=TTC(N)
000021      10 UC(I)=-TUC(N)
000022      NOG=NX+1-NOG
000023      RETURN
000024      END
```

* ELT FLOP,1,710514, 38499 , 1

```
000001      SUBROUTINE FLOP(A,B,C,D,E,NX)
000002      DIMENSION A(41),B(41),C(41),D(41),E(41)
000003      DIMENSION AA(20),BB(20),CC(20),DD(20),EE(20)
000004      DO 10 I=1,NX
000005      AA(I)=A(I)
000006      BB(I)=B(I)
000007      CC(I)=C(I)
000008      DD(I)=D(I)
000009      10 EE(I)=E(I)
000010      DO 20 N=1,NX
000011      I=NX+1-N
000012      A(I)=AA(N)
000013      B(I)=BB(N)
000014      C(I)=CC(N)
000015      D(I)=DD(N)
000016      20 E(I)=EE(N)
000017      RETURN
000018      END
```

* ELT GAST,1,710514, 38500 , 1

```
000001      SUBROUTINE GAST (DX,RHOG,CPG,U,TS,TX,NDX1,ASG,HSG,AXG,HXG,TG,VOIDF
000002      1)
000003      DIMENSION RHOG(1),CPG(1),U(1),TS(1),TX(1),TG(1),ASG(1),HSG(1),HXG(
000004      11),VOIDF(1),AXG(1)
000005      W=1.0
000006      N2= NDX1-1
000007      TG(1)=TS(1)
000008      DO 10 N= 1, N2
000009      F= 0.5*(VOIDF(N)+ VOIDF(N+1))
000010      AS1=ASG(N+1)
000011      HS1=HSG(N+1)
000012      AX1=AXG(N+1)
000013      HX1=HXG(N+1)
000014      CP1=CPG(N)
000015      R0 = 0.5*(RHOG(N)+RHOG(N+1))
000016      U1= 0.5*( U(N)+U(N+1))
000017      TS1=TS(N+1)
000018      TX1=TX(N+1)
000019      C1=1./(F+R0*CP1+U1)
000020      D=C1*(AS1*HS1*TS1*AX1*HX1)
000021      A=(AS1*HS1*AX1*HX1)*C1
000022      10 TG(N+1)=((1./DX-A*(1.-W))*TG(N)+D)/(1./DX+A*W)
000023      RETURN
000024      END
```

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* ELT GASTA,1,710514, 38501 , 1

```

000001      SUBROUTINE GASTA(GMR,CPG,ABED,NDX1,TG1,ASG,HSG,AXG,HXG,DX,TG,TS,TX
000002      1)
000003      C
000004      C      GAS TEMPERATURE CALCULATIONS FOR ABSORPTION
000005      C
000006      DIMENSION CPG(1),ASG(1),HSG(1),HXG(1),TG(1),TS(1),TX(1),ABED(1),
000007      1,AXG(1)
000008      C
000009      TG(NDX1+1) = TG1
000010      DO 10 N=1,NDX1
000011      C=GMR*CPG(N)/ABED(N)
000012      N1=NDX1+1-N
000013      C1=ASG(N1)*HSG(N1)+AXG(N1)*HXG(N1)
000014      10 TG(N1) = (TG(N1+1)/DX+(ASG(N1)*HSG(N1)*TS(N1)+AXG(N1)
000015      *HXG(N1)*TX(N1))/1C)/(1./DX+C1/C)
000016      RETURN
000017      END
000018

```

* ELT HXCORE,1,710719, 62343 , 1

```

000001      SUBROUTINE HXCORE
000002      COMMON/AD/ TG(20),PH201,TG1,PA,PK(2,20),PC021,TS(20)
000003      1,TC(20),TX(20),TS1(20),TS2(20),TX1(20),TX2(20),TC1(20),
000004      2,TC2(20),W(4,20),PT(20),GMR,GMW,GV1S,PN2,P02,
000005      3,ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),
000006      4,AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),
000007      5,CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),
000008      6,POUT(10),TIMET(10),WTACMS,WTSQ,PUMP(10),VPUMP(10),CPP(20),
000009      7,NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20),
000010      8,HXG(20),HXS(20),HXC(20),HSG(20),
000011      9,SK(20),TKX(20),DH(20),DIF(20),GK(20),UC(20),T268,TOTC02,TOTH20,
000012      1,ISUMPTM,AVMSL1,AVSCL1,HTR(20),TMAX,
000013      1,TOTKWH,HTR1(20),WC,TOTHTC,WCC,PC02A,VC02A,SABC02,TC02A,
000014      1,RS1(20),9,A(20),F(20),C(20),VS(20),DVS(20),DVS1(20),RS(20),
000015      1,U(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),
000016      2,D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),
000017      3,F(2,20),P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3
000018      4(20,4),C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),V01DF(20),
000019      5,WM(2),TIME,CYCLE,DT0,DTMAX,WI,TI,PC02C,
000020      6,VOLCAB,RC02C,
000021      7,NCYCLT,NPRINT,NCYCLE,NDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SABCOS
000022      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,
000023      1,C1P,C2P,X,C1P,C2P,C3P,D1P
000024      EQUIVALENCE (NDX,NDX1)
000025      DIMENSION S1(20),S2(20),S3(20),DD(20)
000026      C
000027      DN=DT+DT0
000028      DO 10 N=1,NDX
000029      T1= AVX(N)*(HXC(N)+HXS(N)+HXG(N))*0.5
000030      S1(N)=-TKX(N)/DX/DX
000031      S3(N)= -TKX(N+1)/DX/DX
000032      S2(N)= RHGX(N)*CPX(N)/DN -S1(N) - S3(N) + T1
000033      10 DD(N) = RHGX(N)*CPX(N)/DN*TX2(N) + AVX(N)*(HXC(N)
000034      *TC1(N) + HXS(N)*TS1(V)+HXG(N)*TG(N)) - T1*TX2(N)+HTR(N)/(ABED(N)*
000035      2*ASX(N)/AVX(N)*DX)
000036      S2(1)=S2(1)+S1(1)
000037      S1(1)=0.
000038      S2(NDX)=S2(NDX)+S3(NDX)
000039      S3(NDX)=0.0
000040      CALL FDEQIM(S1,S2,S3,DD,TX,NDX)
000041      RETURN
000042      END

```

* ELT IFN,1,710514, 38502 , 1

```

000001      FUNCTION IFN(N,NDXM)
000002      IFN=1
000003      IF(N.GT.NDXM)IFN=2
000004      RETURN
000005      END
000006      C

```



P ELT LAGIN2,1,710514, 38503 , 1

```

000001      SUBROUTINE LAGIN2(ID,X,NP,ND,X0,Y0,Y)
000002      REVISED FOR FORTRAN IV 8-8-65 S. WONG
000003      DIMENSION X(2), Y(2)
000004      C
000005      ILO=1
000006      IF(X0-X(1))10,16,4
000007      4 IF(X0-X(NP))19,13,7
000008      7 ILO=NP-1
000009      10 IH1=ILO+1
000010      GO TO 46
000011      13 ILO=NP
000012      16 Y0=Y(ILO)
000013      RETURN
000014      19 DO 22 ILO=2,NP
000015      IF(X0-X(ILO))25,16,22
000016      22 CONTINUE
000017      25 IH1=ILO
000018      ILO=IH1-1
000019      IF(ND-2)46,46,28
000020      28 DO 43 I=3,ND
000021      IF(ILO-1)40,40,31
000022      31 IF(IH1-NP)34,37,37
000023      34 IF (2.*X0-X(ILO-1)-X(IH1+1)) 37,37,40
000024      37 ILO=ILO-1
000025      GO TO 43
000026      40 IH1=IH1+1
000027      43 CONTINUE
000028      46 Y0=0.0
000029      PN=1.0
000030      DO 49 I=ILO,IH1
000031      49 PN=PN*(X0-X(I))
000032      DO 58 I=ILO,IH1
000033      P=PN/(X0-X(I))
000034      DO 55 J=ILO,IH1
000035      IF(J-1)52,55,52
000036      52 P=P/(X(I)-X(J))
000037      55 CONTINUE
000038      Y0=Y0+P*Y(I)
000039      58 CONTINUE
000040      RETURN
000041      1 FORMAT (97X,7HLAGIN2 ,I4,E12.5)
000042      END

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• ELT MAIN4B, 1, 710719, 62345 , 1

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000001      C  MAIN PROGRAM FOR ANALYZING 4-BED SYSTEM FOR CO2 RECOVERY
000002
000003      C
000004      COMMON/AD/ TG(20),PH20I ,TGI ,PA ,          PK (2,20),PC02I ,TS (20)    *NEW
000005      1,TC (20),TX (20), TS1 (20),TS2 (20),TX1 (20),TX2 (20),TC1 (20),    *NEW
000006      2TC2 (20),W (4,20),PT (20),          GMR ,GMW,GVIS, PN2,P02,    *NEW
000007      3          ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),    *NEW
000008      4AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),    *NEW
000009      5CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),    *NEW
000010      6POUT(10),TIMET(10),WTACMS,WTSG ,PUMP(10),VPUMP(10),CPP(20),    *NEW
000011      7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORR(20),    *NEW
000012      8          HXC(20),HXS(20),HXC(20),HSG(20),    *NEW
000013      9SK(20),TKX(20),DH(20),DIF(20),GK(20),UC(20),T268,TOTCO2,TOTH20,    *NEW
000014      1SUMPTM,AVMSL1,AVSGL1,HTR(20),TMX,    *NEW
000015      1TOTKWH,HTR1(20),WC,TOTHTC,WCC,PC02A,VC02A,SABC02, TC02A,    *NEW
000016      1RS1(20,9),          A(20),F(20),C(20),VS(20),DVS(20),DVS1(20),RS(20),    *NEW
000017      1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),    *NEW
000018      2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),    *NEW
000019      3FR(2,20),          P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3    *NEW
000020      4(20,4),C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20),    *NEW
000021      5WM(2),TIME,CYCLE,DTO, DTMAX,W1, TI,PC02C,    *NEW
000022      6VOLCAB,RC02C,    *NEW
000023      7NCYCLT,NPRINT,NCYCLE,NDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SABC05    *NEW
000024      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,    *NEW
000025      1          CP1,CP2,X, C1P,C2P,C3P,D1P    *NEW
000026      COMMON   TG1(20),PH20I1,TGI1,PA1,          PK1(2,20),PC02I1 ,TS01(20)    ***-1
000027      1,TC01(20),TX01(20), TS11(20),TS21(20),TX11(20),TX21(20),TC11(20),    *NEW
000028      2TC21(20),W1(4,20),PT1(20),          GMR1,GMW1,GVIS1,PN21,P021    *NEW
000029      COMMON   TG2(20),PH20I2,TGI2,PA2,          PK2(2,20),PC02I2 ,TS02(20)    *NEW
000030      1,TC02(20),TX02(20), TS12(20),TS22(20),TX12(20),TX22(20),TC12(20),    *NEW
000031      2TC22(20),W2(4,20),PT2(20),          GMR2,GMW2,GVIS2,PN22,P022    *NEW
000032      COMMON   TG3(20),PH20I3,TGI3,PA3,          PK3(2,20),PC02I3 ,TS03(20)    *NEW
000033      1,TC03(20),TX03(20), TS13(20),TS23(20),TX13(20),TX23(20),TC13(20),    *NEW
000034      2TC23(20),W3(4,20),PT3(20),          GMR3,GMW3,GVIS3,PN23,P023    *NEW
000035      COMMON   TG4(20),PH20I4,TGI4,PA4,          PK4(2,20),PC02I4 ,TS04(20)    *NEW
000036      1,TC04(20),TX04(20), TS14(20),TS24(20),TX14(20),TX24(20),TC14(20),    *NEW
000037      2TC24(20),W4(4,20),PT4(20),          GMR4,GMW4,GVIS4,PN24,P024    *NEW
000038      COMMON/B1/ RDB(405),IDB(29)
000039      COMMON/B2/RMB(405),IMB(29)
000040      COMMON/B1A/RDBA(260)
000041      COMMON/B1D/RDBD(260)
000042      COMMON/B2A/ RMBA(260)
000043      COMMON/B2D/ RMBD(260)
000044      DIMENSION RB1M(349),RB2M(349),RB3M(349),RB4M(349),RMAIN(11),
000045      1IMAIN(06),KBED(4)
000046      EQUIVALENCE (RB1M(1),TG1(1)),(RB2M(1),TG2(1)),(RB3M(1),TG3(1)),
000047      1(RB4M(1),TG4(1)),(RMAIN(1),WM(1)),(IMAIN(1),NCYCLT)
000048      NAMELIST/MAIN/ WM, CYCLE,DTMAX,W1, TI,PC02C,VOLCAB,RC02C,
000049      1NPRINT,NDTCON,NTEMP,          TGC,PAC,PH20C,TGHX
000050      2,PC02A,VC02A,SABC02,TC02A,KBED,TIMEDS, NCT1, NST1, NCT2, NST2
000051      NAMELIST/B1M/          PA1,          TS01,TC01,TX01,W1,
000052      1GMR1,GMW1,          PN21,P021
000053      NAMELIST/B2M/          PA2,          TS02,TC02,TX02,W2,
000054      1GMR2,GMW2,          PN22,P022
000055      NAMELIST/B3M/          PA3,          TS03,TC03,TX03,W3,
000056      1GMR3,GMW3,          PN23,P023
000057      NAMELIST/B4M/          PA4,          TS04,TC04,TX04,W4,
000058      1GMR4,GMW4,          PN24,P024
000059      DATA PT2,PT4/ 40*3.0/X/20*1./,C/20*0.2E-3/

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000059      DATA DTT/4*1./
000060      1 CONTINUE          * TO READ IN DATA FOR A NEW PROBLEM
000061      10H FORMAT(13A6,A2)
000062      109 FORMAT(20X,13A6,A2)
000063      READ(5,MAIN)
000064      WRITE(6,MAIN)
000065      READ(5,B1M)
000066      WRITE(6,B1M)
000067      READ(5,B2M)
000068      WRITE(6,B2M)
000069      READ(5,B3M)
000070      WRITE(6,B3M)
000071      READ(5,B4M)
000072      WRITE(6,B4M)
000073      CALL READ1
000074      CALL READ2
000075      CALL READ3
000076      CALL READ4
000077      SABCOS=SABC02
000078      NHALF=1
000079      DO 102 N= 1, 20
000080      TC11(N)=TC01(N)
000081      TC21(N)=TC01(N)
000082      TX11(N)=TX01(N)
000083      TX21(N)=TX01(N)
000084      TS11(N)=TS01(N)
000085      TS21(N)=TS01(N)
000086      TC12(N)=TC02(N)
000087      TC22(N)=TC02(N)
000088      TX12(N)=TX02(N)
000089      TX22(N)=TX02(N)
000090      TS12(N)=TS02(N)
000091      TS22(N)=TS02(N)
000092      TC13(N)=TC03(N)
000093      TC23(N)=TC03(N)
000094      TX13(N)=TX03(N)
000095      TX23(N)=TX03(N)
000096      TS13(N)=TS03(N)
000097      TS23(N)=TS03(N)
000098      TC14(N)=TC04(N)
000099      TC24(N)=TC04(N)
000100      TX14(N)=TX04(N)
000101      TX24(N)=TX04(N)
000102      TS14(N)=TS04(N)
000103      TS24(N)=TS04(N)
000104      102 CONTINUE
000105      NCYCLT=NCT1
000106      NSTART=NST1
000107      ASSIGN 103 TO NSUB4B
000108      GO TO 104
000109      103 CONTINUE
000110      CALL BED4(1.0,3,RB1M,RDR,1DB,RDBA,ISTOPC,KBED)
000111      CALL BED4(2.0,3,RB2M,RMB,IMB,RMBA,ISTOPC,KBED)
000112      DO 201 K=1,60
000113      N=K+120
000114      RMBD(N)=RMBA(N)
000115      RDDB(N)=RDBA(N)
000116      201 CONTINUE
000117      NCYCLT=NCT2
000118      NSTART=NST2

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000119      ASSIGN 105 TO NSUB4B
000120      GO TO 104
000121      105 CONTINUE
000122      CALL EXIT
000123      C
000124      C
000125      104 CONTINUE
000126      C      START SUB4B
000127      NCYCLE=1
000128      101 CONTINUE
000129      IF(NCYCLE .GT. NCYCLT) GO TO NSUB4B
000130      TIME = 0.0
000131      DTO =0.0
000132      DT=1.E-5
000133      NPR = 1
000134      GO TO 3
000135      4 CONTINUE
000136      GO TO ( 3,42),NDTCON
000137      42 DT=DTMAX/10.0
000138      IF(TIME .LT. 1.E-4) DT=DTMAX/1000.0
000139      IF(TIME .GT. 0.06) DT=DTMAX
000140      GO TO 5
000141      3 CONTINUE
000142      DT=AMIN1(DTT(1),DTT(2),DTT(3),DTT(4))
000143      IF(TIME .LT. 8.E-5) DT=1.E-5
000144      5 IF((TIME+DT) .GT. CYCLE) DT = CYCLE-TIME
000145      TIME=TIME+DT
000146      GO TO(20,21), NHALF
000147      C *****PART TO BE CHANGED FOR DIFFERENT HOOK-UP OF SYSTEM *****
000148      C FIRST HALF CYCLE
000149      20 CONTINUE
000150      PC02I1=PC02C
000151      PH20I1=PH20C
000152      TGI1=TGC
000153      ISTOPC=0
000154      CALL BED4(1,0,1,RB1M,RDB,IDB,RDBA,ISTOPC,KBED)
000155      PC02I2=PK (1,1)
000156      PH20I2=PK (2,1)
000157      TGI2=TG (1)
000158      IF(TG1(1) .GT. TGWX) TGI2=TGHX
000159      RMB(201)=TC01(10)
000160      35 CALL BED4(2,0,1,RB2M,RMB,IMB,RMBA,ISTOPC,KBED)
000161      DPC02C=UT*(RC02C-GMR*(PC02C-PK2(1,1))*44./          (PA*GMW))*554.*530./
000162      (44.*VOLCAB)
000163      IF((KBED(1).EQ.0),AND.(KBED(2).EQ.0))DPC02C=0.
000164      PC02C=PC02C+DPC02C
000165      PC02I3=PK (1,1)
000166      PH20I3=0.00000
000167      TGI3=TG (1)
000168      IF(TIME.GT.TIMEDS) ISTOPC=1
000169      CALL BED4(3,1,1,RB3M,RDB,IDB,RDBD,ISTOPC,KBED)
000170      RMBD(201)=TC03(10)
000171      CALL BED4(4,0,2,RB4M,RMB,IMB,RMBD,ISTOPC,KBED)
000172      C ***** TO BE CHANGED UP TO HERE *****
000173      NPR = NPR+1
000174      DTO=DT
000175      IF(TIME .GE. CYCLE) NHALF=2
000176      IF(TIME .GE. CYCLE) GO TO 101
000177      GO TO 4
000178      C *****PART TO BE CHANGED FOR DIFFERENT HOOK-UP OF SYSTEM *****

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000179      C SECOND HALF CYCLE
000180      21 CONTINUE
000181      ISTOPC=0
000182      PC02I3=PC02C
000183      PH20I3=PH20C
000184      TG13=TGC
000185      CALL BED4(3,0,1,RB3M,RDB,I0B,RDRA,ISTOPC,KBED)
000186      PC02I4=PK (1,1)
000187      PH20I4=PK (2,1)
000188      TG14=TG (1)
000189      IF(TG3(1) .GT. TGHX) TG14=TGHX
000190      RMBA(201)=TC03(10)
000191      36 CALL BED4(4,0,1,RB4M,RMB,IMB,RMBA,ISTOPC,KBED)
000192      DPC02C=DT*(RC02C-GMR*(PC02C-PK4(1,1))*44./ (PA*GMW))*554.*530./
000193      1(44.*VOLCAB)
000194      IF((KBED(3).EQ.0),AND.(KBED(4).EQ.0))DPC02C=0.
000195      PC02C=PC02C+DPC02C
000196      PC02I1=PK (1,1)
000197      PH20I1=0.0000
000198      TG11=TG (1)
000199      IF(TIME.GT.TIMEDS) ISTOPC=1
000200      CALL BED4(1,1,1,RB1M,RDB,I0B,RDBD,ISTOPC,KBED)
000201      RMBD(201)=TC01(10)
000202      CALL BED4(2,0,2,RB2M,RMB,IMB,RMBD,ISTOPC,KBED).
000203      C ***** TO BE CHANGED UP TO HERE *****
000204      NPR = NPR+1
000205      DTO=DT
000206      IF(TIME .GE. CYCLE) NHALF=1
000207      IF(TIME.GE.CYCLE) NCYCLE=NCYCLE+1
000208      IF(TIME.GE. CYCLE) GO TO 101
000209      GO TO 4
000210      END

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* ELT NEWTO2,1,710609, 32711 , 1

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000001      SUBROUTINE NEWTO2(N1,NGO,X,Y,X0,Y0,XMIN,XMAX,ER)
000002      C   SET N1=1 IN MAIN PROGRAM BEFORE CALL NEWTON. THE ROUTINE
000003      C   FINDS X FOR Y=0 GIVES NGO=1 IF RECALCULATIONS REQUIRED.
000004      C   GIVES NGO=2 IF CONVERGENCE REACHED.
000005      N1=N1-1
000006      IF( ABS(Y)-ER) 8,8,5
000007      5 IF(N1)7,6,7
000008      6 Y0=Y
000009      X0=X
000010      X=X0+(XMAX-XMIN)*0.01
000011      IF(X-XMAX)21,21,14
000012      14 X=X0-(XMAX-XMIN)*0.01
000013      GO TO 21
000014      7 SLOPE=(Y-Y0)/(X-X0)
000015      Y0=Y
000016      X0=X
000017      X=X-Y/SLOPE
000018      IF(N1+8)20,20,21
000019      20 X=0.5*(X+X0)
000020      IF(N1+20)22,22,21
000021      22 WRITE (6,23)
000022      WRITE (6,30) X,Y,X0,Y0,ER
000023      23 FORMAT (32HDEEXCEED 20 ITERATIONS IN NEWTON //)
000024      N1=0
000025      ER=5.*ER
000026      21 CONTINUE
000027      IF(X-XMIN)11,11,12
000028      11 X=XMIN
000029      IF(X-X0)9,8,9
000030      12 IF(X-XMAX)9,13,13
000031      13 X=XMAX
000032      IF(X-X0)9,8,9
000033      9 NGO=1
000034      RETURN
000035      8 NGO=2
000036      N1=1
000037      RETURN
000038      30 FORMAT(14H X,Y,X0,Y0,ER= 5G14.4)
000039      END

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* ELT PRA05B, 710719, 62347 , 1

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000001      SUBROUTINE PRA05B(1BED)          *NEW
000002      C
000003      COMMON/AD/ TG(20),PH201,TG1,PA,      PK(2,20),PC021,TS(20)   *NEW
000004      1,TC(20),TX(20),TS1(20),TS2(20),TX1(20),TX2(20),TC1(20),   *NEW
000005      2,TC2(20),W(4,20),PT(20),      GMR,GMW,GVIS,PN2,P02,   *NEW
000006      3,ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),   *NEW
000007      4,AVX(20),RHOG(20),RHOS(20),RHOS(20),RHOC(20),RHOX(20),   *NEW
000008      SCPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),   *NEW
000009      6POUT(10),TIMET(10),WTACMS,WTSG,PUMP(10),VPUMP(10),CPF(20),   *NEW
000010      7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20),   *NEW
000011      8,HXG(20),HXS(20),HXC(20),HSG(20),   *NEW
000012      9SK(20),TKX(20),DH(20),DIF(20),GK(20),UC(20),T268,TOTCO2,TOTH20,   *NEW
000013      1,SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX,   *NEW
000014      1,TOTKWH,HTR1(20),WC,TOTHTC,WCC,PC02A,VC02A,SABC02,TC02A,   *NEW
000015      1,RS1(20,9),A(20),F(20),C(20),VS(20),DVS(20),DVS1(20),RS(20),   *NEW
000016      1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),   *NEW
000017      2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),   *NEW
000018      3FR(2,20),P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3   *NEW
000019      4(20,4),C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20),   *NEW
000020      5,WM(2),TIME,CYCLE,DTO,DTMAX,WI,TI,PC02C,   *NEW
000021      6,VOLCAE,RC02C,   *NEW
000022      7,NCYCLT,NPRINT,NCYCLE,NDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SABC05   *NEW
000023      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,   *NEW
000024      1,CP1,CP2,X,C1P,C2P,C3P,D1P   *NEW
000025      C
000026      DIMENSION AVLD(41)           **-1
000027      EQUIVALENCE(NDX,NDX1)
000028      AVMSLD=0.0
000029      AVSGLD=0.0
000030      AVRCD02=0.0
000031      AVRHD20=0.0
000032      AVPH20 = SUMPTM/TIME
000033      AVH20P=GMR*AVPH20*18./(PA*GMW)
000034      C
000035      TIMEM=60.*TIME
000036      WRITE(6,499)IBED
000037      WRITE(6,100) NCYCLE,TIME ,TIMEM,DT
000038      WRITE(6,101)
000039      WRITE(6,102)(N,PK(1,N),PK(2,N),
000040      1,TG(N),TS(N),TC(N),TX(N),N=1,NDX)
000041      WRITE(6,103)PK(1,NDX1+1),PK(2,NDX1+1),TG(NDX1+1)
000042      103 FORMAT(' INLET' F10.4,F12.4,F19.4)
000043      WRITE(6,202)
000044      N1=NDXM+1
000045      NDR3=NDR4-1
000046      DO 20 N= 1, NDXM
000047      SUMMS=0.0
000048      SUMMS=SUMMS+0.5*(W(1,N)+W(NDR4,N))
000049      IF(NDR4.EQ.2) AVLD(N) = SUMMS
000050      IF(NDR4.EQ.2) GO TO 20
000051      DO 22 NR=2,NDR3
000052      22 SUMMS=SUMMS+W(NR,N)
000053      AVLD(N)=SUMMS/NDR3
000054      20 CONTINUE
000055      DO 30 N= N1,NDX1
000056      SUMMS=0.0
000057      SUMMS=SUMMS+0.5*(W(1,N)+W(NDR4,N))
000058      IF(NDR4.EQ.2) AVLD(N) = SUMMS

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000059      IF(NDR4.EQ.2) GO TO 30
000060      DO 33 NR=2, NDR3
000061      SUMMS=SUMMS+W(NR,N)
000062      AVLD(N)=SUMMS/NDR3
000063      30 CONTINUE
000064      SUM=0.
000065      IF(NDXMAC .EQ. 0) GO TO 35
000066      DO 31 N= 1, NDXMAC
000067      31 SUM= SUM+AVLD(N)*ABED(N)*DX*RHOSE(N)
000068      AVMSLD = SUM/WTACMS
000069      SUM=0.
000070      35 CONTINUE
000071      IF((NDX1-NDXM).EQ. 0) GO TO 40
000072      DO 32 N= N1,NDX1
000073      32 SUM = SUM+AVLD(N)*ABED(N)*DX*RHOSE(N)
000074      AVSGLD=SUM/WTSG
000075      40 CONTINUE
000076      DO 10 N=1,NDX
000077      10 WRITE (6,203)N, AVLD(N)
000078      1          ,(W(NR,N),NR=1,NDR4)
000079      IF(TIME .LT. 1.1E-5) AVMSL1=AVMSLD
000080      IF(TIME .LT. 1.1E-5) AVSGL1=AVSGLD
000081      AVRCD2=WTACMS*(AVMSLD-AVMSL1)/TIME
000082      AVRHD2=WTSG*(AVSGLD-AVSGL1)/TIME
000083
C      DIMENSION F1(9),F2(9),F3(9),F4(9), F5(9),F6(9),F7(9)
000084      WRITE(6,205) F1,AVMSLD,F2,AVSGLD,F3,AVRC02,F4,AVRH20,F5,TOTKWH,
000085      1F6,TOTHTC,F7,AVPH20
000086      205 FORMAT(///(9A6,F8.4,6X,9A6,F8.4))
000087      DATA F1//' AVG CO2 LOADING IN C02 SORBENT (LB/LB)'/'
000088      DATA F2//' AVG H2O LOADING IN DESCANT (LB/LB)'/'
000089      DATA F3//' TIME AVG CO2 ADSORPTION RATE (LR/HR)'/'
000090      DATA F4//' TIME AVG H2O ADSORPTION RATE (LR/HR)'/'
000091      DATA F5//' ELECTRICAL HEAT INPUT FROM START OF CYCLE (KWH)'/'
000092      DATA F6//' HEAT ADDED BY COOLANT FROM START OF CYCLE (BTU)'/'
000093      DATA F7//' TIME AVG OUTLET PH20 (MM)'/'
000094
C      RETURN
000095
000096
000097      499 FORMAT(8H1BED NO. 13)
000098      100 FORMAT (1H0,16HADSORPTION CYCLE 13/
000099      1          3X,5HTIME=,F9.5,1X2HHR,F12.3,1X,3HMIN,
000100      1          5X,15HTIME INCREMENT=F7.5,1X2HHR)
000101      101 FORMAT (//2X,10HAXIAL NODE,3X,7HPC02,MM,5X,7HPH20,MM,8X,
000102      1          11HGAS TEMP, F
000103      1          ,8X,15HSORBENT TEMP, F     ,6X,15HCOOLANT TEMP, F   ,7X,15HGX CO
000104      2RE TEMP, F )
000105      102 FORMAT(/(19.2F12.4,5X,4(F14.4,6X)))
000106      202 FORMAT (// 38HLOADING AT INTERIOR OF SORBENT, LB/LB
000107      1          //4X,4HSORB/4X,4HNOD
000108      1E,3X, 3HAVG, 9X,
000109      1          1H1,9X,1H2,9X,1H3,9X,1H4
000110      2          /6H AXIAL/BH NODE)
000111      203 FORMAT ( 15,4X,12(F6.4,4X))
000112      END

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* ELT PRDESB, 1, 710719, 62348 , 1

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000001      SUBROUTINE PRDESB(1BED)
000002
000003
000004      COMMON/AD/ TG(20),PH20I ,TGI ,PA ,      PK (2,20),PC02I ,TS (20) *NEW
000005      1,TC (20),TX (20), TS1 (20),TS2 (20),TX1 (20),TX2 (20),TC1 (20), *NEW
000006      2TC2 (20),W (4,20),PT (20),      GMR ,GMW,GVIS, PN2,P02, *NEW
000007      3 ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20), *NEW
000008      4AVX(20),RHOG(20),RHOS(20),RHOS(20),RHOC(20),RHOX(20), *NEW
000009      5CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20), *NEW
000010      6POUT(10),TIMET(10),WTACMS,WTSC ,PUMP(10),VPUMP(10),CPP(20), *NEW
000011      7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20), *NEW
000012      8 HXG(20),HXS(20),HXC(20),HSG(20), *NEW
000013      9SK(20),TKX(20),DH(20),DIF(20),GK(20),UC(20),T268,TOTCO2,TOTH20, *NEW
000014      1SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX, *NEW
000015      1 TOTKWH,HTR1(20),WC,TOTHTC,WCC,PC02A,VC02A,SARC02, TC02A, *NEW
000016      1RS1(20,9), A(20),F(20),C(20),VS(20),DVS(20),DVS1(20),RS(20), *NEW
000017      1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20), *NEW
000018      2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20), *NEW
000019      3FR(2,20), P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3 *NEW
000020      4(20,4), C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20), *NEW
000021      5 WM(2),TIME,CYCLE,DT0, DTMAX,WI,TI,PC02C, *NEW
000022      6VOLCAB,RC02C, *NEW
000023      7NCYCLT,NPRINT,NCYCLE,NDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SABC05 *NEW
000024      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B, *NEW
000025      1 CP1,CP2,X, C1P,C2P,C3P,D1P *NEW
000026      DIMENSION AVLD(41), *NEW
000027      EQUIVALENCE(NDX,NDX1). **-1
000028
000029
000030      AVMSLD=0.0
000031      AVSGLD=0.0
000032      AVR02=0.0
000033      AVRH20=0.0
000034      TIMEM=60.*TIME
000035      WRITE(6,499)1BED
000036      WRITE(6,100) NCYCLE,TIME ,TIMEM,DT
000037      WRITE (6,102)(N,PT(N),TG(N),TS(N),TC(N),TX(N),N=1,NDX)
000038      IF(( NPSET(1) .GT. 0 ) .OR. (NPSET(2) .GT. 0 )) GO TO 99
000039
000040      99 WRITE (6,202)
000041      N1=NDXM+1
000042      NDR3=NDR4-1
000043      DO 20 N= 1, NDXM
000044      SUMMS=0.0
000045      SUMMS=SUMMS+0.5*(W(1,N)+W(NDR4,N))
000046      IF(NDR4 .EQ. 2) AVLD(N) = SUMMS
000047      IF(NDR4.EQ.2) GO TO 20
000048      DO 22 NR=2,NDR3
000049      22 SUMMS=SUMMS+W(NR,N)
000050      AVLD(N)=SUMMS/NDR3
000051
000052      20 CONTINUE
000053      DO 30 N= N1,NDX1
000054      SUMMS=0.0
000055      SUMMS=SUMMS+0.5*(W(1,N)+W(NDR4,N))
000056      IF(NDR4.EQ.2) AVLD(N) = SUMMS
000057      IF(NDR4.EQ.2) GO TO 30
000058      DO 33 NR=2, NDR3
000059      33 SUMMS=SUMMS+W(NR,N)
000060      AVLD(N)=SUMMS/NDR3

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000059      30 CONTINUE
000060      IF(NDXMAC .EQ. 0) GO TO 35
000061      SUM=0.
000062      DO 31 N= 1, NDXMAC
000063      SUM= SUM+AVLD(N)*ABED(N)*DX*RHOSB(N)
000064      AVMSLD = SUM/WTACMS
000065      35 CONTINUE
000066      IF((NDX1-NDXM) .EQ. 0) GO TO 40
000067      SUM=0.
000068      DO 32 N= N1,NDX1
000069      SUM = SUM+AVLD(N)*ABED(N)*DX*RHOSB(N)
000070      AVSGLD=SUM/WTSG
000071      40 CONTINUE
000072      DO 10 N=1,NOX
000073      10 WRITE (6,203)N, AVLD(N)
000074      1      ,(W(NR,N),NR=1,NDR4)
000075      IF(TIME .LT. 1.1E-5) AVMSL1=AVMSLD
000076      IF(TIME .LT. 1.1E-5) AVSGL1=AVSGLD
000077      AVRCo2=WTACMS*(AVMSL1-AVMSLD)/TIME
000078      AVRH20=WTSG*(AVSGL1-AVSGLD)/TIME
000079      DIMENSION F1(9),F2(9),F3(9),F4(9), F5(9),F6(9),F7(9),F8(9),F9(9)
000080      WRITE(6,205) F1,AVMSLD,F2,AVSGLD,F3,AVRC02,F4,AVRH20,F5,TOTKWH,
000081      1F6,TOTHTC,          FB,PC02A, F9,VC02A
000082      205 FORMAT(////(9A6,F8.4,6X,9A6,F8.4))
000083      DATA F1//' AVG CO2 LOADING IN CO2 SORBENT (LB/LB)''/
000084      DATA F2//' AVG H2O LOADING IN DESICCANT (LB/LB)''/
000085      DATA F3//' TIME AVG CO2 DESORPTION RATE (LB/HR)''/
000086      DATA F4//' TIME AVG H2O DESORPTION RATE (LB/HR)''/
000087      DATA F5//' ELECTRICAL HEAT INPUT FROM START OF CYCLE (KWH)''/
000088      DATA F6//' HEAT ADDED BY COOLANT FROM START OF CYCLE (BTU)''/
000089      DATA F7//' CABIN CO2 PARTIAL PRESSURE (MM)''/
000090      DATA F8//' ACCUMULATOR CO2 PRESSURE (PSIA)''/
000091      DATA F9//' CO2 ACCUMULATOR VOLUME (CU FT)''/
000092
000093      499 FORMAT(8H1BED NO. 13)
000094      100 FORMAT (1H0,16HDESORPTION CYCLE 13/
000095      1      3X,5HTIME=.F9.5,1X2HHR,F12.3,1X,3HMIN,
000096      1      5X,15HTIME INCREMENT=F7.5,1X2HHR)
000097      101 FORMAT (//2X,10HAXIAL NODE,10X,14HTOTAL PRESS,MM,6X,14HGAS TEMP,DE
000098      1G F,5X,19HSORBENT TEMP, DEG F,2X,18HCoolant TEMP,DEG F,3X,19HHX CO
000099      2RE TEMP, DEG F )
000100      102 FORMAT (/(I9,11X,5(F14.4,6X)))
000101      103 FORMAT ( /21HCO2 DESORPTION RATE=F7.4,1X5HLB/HR,5X,20HH2O DESORPTI
000102      1ON RATE=F7.4,1X5HLB/HR)
000103      200 FORMAT (1H0/2X,10HAXIAL NODE,13X,9HMOLE FRAC,7X,
000104      12X,13HCO2 RATE,M/HR,6X,13HH2O RATE,M/HR)
000105      201 FORMAT (/(I9,11X,3(4X,F12.6,4X)))
000106      202 FORMAT (// 31HOLOADING AT INTERIOR OF SORBENT//4X,4HSORB/4X,4HNOD
000107      1E,3X, 3HAVG, 9X,
000108      1      1H1,9X,1H2,9X,1H3,9X,1H4
000109      2      /6H AXIAL/5H NODE)
000110      203 FORMAT ( 15.4X,12(F6.4,4X))
000111      RETURN
000112      END

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@ ELT READ1,1,710712, 56801 , 1

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000001      SUBROUTINE READ1
000002      COMMON/B1/
000003      1          ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),
000004          2AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),
000005          3CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),
000006          4POUT(10),TIMET(10),WTACMS,WTSG,PUMP(10),VPUMP(10),CPP(20),
000007          5          NPSET(3),VDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20)
000008      COMMON/B1A/
000009      1          HXG(20),HXS(20),HXC(20),HSG(20),
000010      2SK(20),TKX(20),DH(20),DIF(20),GK(20),UC(20),T268,TOTC02,TOTH20,
000011      3SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX
000012      1,TOTKWH,HTR1(20),WC,TOTHTC,WCC,PC02A,VC02A,SABC02,TC02A
000013      NAMELIST/DB / ABED,AVC, ASX,AGX, AVX,RHOG,RHOSB,RHOS,RHOC,
000014      1RHOX,CPG, CPC,CPX,CPP,DX,NPSET,NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,
000015      2POUT,TIMET, PUMP,VPUMP,IDSORB,CPL,DP
000016      NAMELIST/DBA / HXG,HXS,HXC,HSG,SK,TKX,DH,DIF,GK, TCIN,HTR1,TMAX
000017      1,WCC
000018      EQUIVALENCE(TCIN,T268)
000019      READ(5,DB)
000020      WRITE(6,DB)
000021      READ(5,DBA)
000022      WRITE(6,DBA)
000023      DO 10 N=1,NDX1
000024      10 ASG(N)=6.*RHOSB(N)/RHOS(N)/DP(N)
000025      RETURN
000026      END

```

@ ELT READ2,1,710712, 56801 , 1

```

000001      SUBROUTINE READ2
000002      COMMON/B1D/
000003      1          HXG(20),HXS(20),HXC(20),HSG(20),
000004      2SK(20),TKX(20),DH(20),DIF(20),GK(20),UC(20),T268,TOTC02,TOTH20,
000005      3SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX
000006      1,TOTKWH,HTR1(20),WC,TOTHTC,WCC,PC02A,VC02A,SABC02,TC02A
000007      NAMELIST/DBD / HXG,HXS,HXC,HSG,SK,TKX,DH,DIF,GK, TCIN,HTR1,TMAX
000008      1,WCC
000009      EQUIVALENCE(TCIN,T268)
000010      READ(5,DBD)
000011      WRITE(6,DBD)
000012      RETURN
000013      END

```

@ ELT READ3,1,710712, 56802 , 1

```

000001      SUBROUTINE READ3
000002      COMMON/B2/
000003      1          ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),
000004          2AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),
000005          3CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),
000006          4POUT(10),TIMET(10),WTACMS,WTSG,PUMP(10),VPUMP(10),CPP(20),
000007          5          NPSET(3),VDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20)
000008      COMMON/B2A/
000009      1          HXG(20),HXS(20),HXC(20),HSG(20),
000010      2SK(20),TKX(20),DH(20),DIF(20),GK(20),UC(20),T268,TOTC02,TOTH20,
000011      3SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX
000012      1,TOTKWH,HTR1(20),WC,TOTHTC,WCC,PC02A,VC02A,SABC02,TC02A
000013      NAMELIST/MB / ABED,AVC, ASX,AGX, AVX,RHOG,RHOSB,RHOS,RHOC,
000014      1RHOX,CPG, CPC,CPX,CPP,DX,NPSET,NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,
000015      2POUT,TIMET, PUMP,VPUMP,IDSORB,CPL,DP
000016      NAMELIST/MBA / HXG,HXS,HXC,HSG,SK,TKX,DH,DIF,GK, TCIN,HTR1,TMAX
000017      1,WCC
000018      EQUIVALENCE(TCIN,T268)
000019      DATA RHCG/ 20*0.0003/
000020      READ(5,MB)
000021      WRITE(6,MB)
000022      READ(5,MBA)
000023      WRITE(6,MBA)
000024      DO 10 N=1,NDX1
000025      10 ASG(N)=6.*RHOSB(N)/RHOS(N)/DP(N)
000026      RETURN
000027      END

```



* ELT READ4,1,710712, 56803 , 1

```
000001      SUBROUTINE READ4
000002      COMMON/B2D/
000003      1          HXG(20),HXS(20),HXC(20),HSG(20),
000004      2SK(20),TKX(20),DH(20),DIF(20),GK(20),UC(20),T268,TOTC02,TOTH20,
000005      3SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX
000006      1,TOTKWH,HTR1(20),WC,TOTHTC,WCC,PC02A,VC02A,SABC02,TC02A
000007      NAMELIST/MBD / HXG,HXS,HXC,HSG,SK,TKX,DH,DIF,GK,   TCIN,HTR1,TMAX
000008      1,WCC
000009      EQUIVALENCE(TCIN,T268)
000010      READ(5,MBD)
000011      WRITE(6,MBD)
000012      RETURN
000013      END
```

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* ELT START, 1.710719, 62350 1

```

000001      SUBROUTINE START
000002      C
000003      COMMON/AD/ TG(20),PH20I ,TGI ,PA ,      PK (2,20),PC02I ,TS (20)      *NEW
000004      1,TC (20),TX (20),TS1 (20),TS2 (20),TX1 (20),TX2 (20),TC1 (20),      *NEW
000005      2TC2 (20),W (4,20),PT (20),      GMR ,GMW,GVIS ,PN2,P02,      *NEW
000006      3      ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),      *NEW
000007      4AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),      *NEW
000008      5CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),      *NEW
000009      6POUT(10),TIMET(10),WTACMS,WTSG ,PUMP(10),VPUMP(10),CPP(20),      *NEW
000010      7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDS0RR(20),      *NEW
000011      8      HXG(20),HKS(20),HXC(20),HSG(20),      *NEW
000012      9SK(20),TKX(20),DH(20),DIF(20),GK(20) ,UC(20),T268,TOTCO2,TOTH20,      *NEW
000013      1SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX,      *NEW
000014      1 TOTKWH,HTR1(20),WC,TOTHTC,WCC,PC02A,VC02A,SABC02, TC02A,      *NEW
000015      1RS1(20,9),      A(20),F(20),C(20),VS(20),DVS(20),DVS1(20),RS(20),      *NEW
000016      1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),      *NEW
000017      2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),      *NEW
000018      3FR(2,20),      P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3      *NEW
000019      4(20,4),      C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20),      *NEW
000020      5      WM(2),TIME,CYCLE,DTO,      DTMAX,WI,TI,PC02C,      *NEW
000021      6VOLCAB,RC02C,      *NEW
000022      7NCYCLT,NPRINT,NCYCLE,NDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SARCOS      *NEW
000023      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,0,B,      *NEW
000024      1      CP1,CP2,X,      C1P,C2P,C3P,D1P      *NEW
000025      C
000026      DO 5 N=1,NDX1
000027      I=IFN(N,NDXM)
000028      CPS(N)=CPP(N)+W(1,N)*CPL(I)
000029      5 RS(N)=DP(N)/2.000
000030      DO 30 N= 1, NDX1
000031      30 VOIDF(N) = 1. - RHOSB(N)/RHOS(N)
000032      DO 115 N=1,NDX1
000033      115 A(N)= GMR/ABED(N)/PA/GMW
000034      NDR=NDR4-1.
000035      NDR2= 2*NDR
000036      NDR3=NDR2+1
000037      DO 10 I=1,NDX1
000038      VS(I)=4./3.*3.1416*RS(I)**3
000039      DVS(I)=VS(I)/NDR
000040      DVS1(I)=DVS(I)/2
000041      RS1(I,1)=0.
000042      DO 10 K=2,NDR3.
000043      10 RS1(I,K)=CBRT(3./4./3.1416*(4./3.*3.1416*RS1(I,K-1)**3+DVS1(I)))
000044      DO 11 I=1,NDX1
000045      CR1(I,1)=DVS1(I)*RHOS(I)
000046      CR2(I,1)=0.
000047      CR3(I,1)=4.*3.1416*RS1(I,2)**2*DIF(I)/(RS1(I,3)-RS1(I,1))*RHOS(I)
000048      DO 11 K=2,NDR4
000049      CR1(I,K)=DVS(I)*RHOS(I)
000050      CR2(I,K)=4.*3.1416*RS1(I,2*K-2)**2*DIF(I)/(RS1(I,2*K-1)-RS1(I,2*K-3))*RHOS(I)
000051      11 CR3(I,K)=4.*3.1416*RS1(I,2*K)**2*DIF(I)/(RS1(I,2*K+1)-RS1(I,2*K-1)
000052      1)*RHOS(I)
000053      DO 12 N=1,NDX1
000054      12 CR1(N,NDR4)=CR1(N,1)
000055      RETURN
000056      END
000057

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* ELT TGLCOL, 1.710514, 58260 , 1

```

000001      SUBROUTINE TGLCOL(TC,NDXMAX,UC,RHOC,CPC,CX,AXC,HXC,T268,TX,DX,DT,
000002        1AVC, NOGLIN,DT0,TS1,TS2,TX1,TX2,TC1,TC2)
000003        DIMENSION C1(20),C2(20),C3(20),D(20),TC(1),TX(1),HXC(1),AVC(1),
000004          1      TS1(1),TS2(1),TX1(1),TX2(1),TC1(1),TC2(1)
000005        DIMENSION UC(1),RHOC(1),CPC(1),AXC(1)
000006        DN=DT+DT0
000007        DO 10 N=1,NDXMAX
000008          CC1=-UC(N)
000009          CC2=HXC(N)/(CPC(N)*RHOC(N))*AVC(N)*0.5
000010          IF( UC(N) .GT. 0.) GO TO 5
000011          C3(N)=-CC1/DX
000012          C2(N)=1./DN+CC2-C3(N)
000013          C1(N)=0.0
000014          GO TO 10
000015          5 C1(N) = CC1/DX
000016          C2(N) = 1./DN + CC2 - C1(N)
000017          C3(N) = 0.0
000018          10 D(N)=TC2(N)/DN+CC2*TX1(N)*2. - CC2*TC2(N)
000019          C1(NOGLIN) = 0.
000020          C3(NOGLIN) = 0.
000021          D(NOGLIN)=D(NOGLIN) + ABS(UC(NOGLIN))/DX*T268
000022          CALL FDEQIM(C1,C2,C3,D,TC,NDXMAX)
000023          RETURN
000024          END

```

* ELT TSORB, 1.710719, 62351 , 1

```

000001      SUBROUTINE TSORB
000002      COMMON/AD/ TG(20),PH201,TG1,PA,PK(2,20),PC021,TS(20)
000003      1/TC(20),TX(20),TS1(20),TS2(20),TX1(20),TX2(20),TC1(20),
000004      2TC2(20),W(4,20),PT(20),GMR,GMW,GVIS,PN2,P02,
000005      3      ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),
000006      4AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),
000007      5CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),
000008      6POUT(10),TIMET(10),WTACMS,WTSG,PUMP(10),VPUMP(10),CPP(20),
000009      7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20),
000010      8      HXG(20),HXS(20),HXC(20),HSG(20),
000011      9SK(20),TKX(20),DH(20),DIF(20),GK(20),UC(20),T268,TOTCO2,TOTH20,
000012      1SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX,
000013      1      TOTKHN,HTR1(20),WC,TOTHTC,WCC,PC02A,VC02A,SABC02,TC02A,
000014      1RB1(20,9),A(20),F(20),C(20),VS(20),DVS(20),DVS1(20),RS(20),
000015      1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),
000016      2D2(20),PC1(20),PC2(20),C1P(20),C2P(20),C3P(20),D1P(20),
000017      3FR(2,20),P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3
000018      4(20,4),C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20),
000019      5      WM(2),TIME,CYCLE,DT0,DTMAX,WI,TI,PC02C,
000020      6VOLCAB,RC02C,
000021      7NCYCLT,NPRINT,NCYCLE,NDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SABC05
000022      DOUBLE PREC18ION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,
000023      1      CP1,CP2,X,C1P,C2P,C3P,D1P
000024      DIMENSION S1(41),S2(41),S3(41),B1(41)      ***-1
000025      DO 10 N=1,NDX1
000026      T=(DT+DT0)/CPS(N)/RHOSB(N)
000027      T1=0.5*T*(ASG(N)*HSG(N)+ASX(N)*HXS(N))
000028      CS1(N)=CS1(N)*(1.0+T1)
000029      CS2(N)=CS2(N)*(1.0+T1)
000030      B1(N)=TS2(N)*CS1(N)*PT(N)-CS2(N)*(P1(N)+P2(N)*(W(NDR4,N)-WS(N))+  
1P3(N)*PT(N))+T*(ASG(N)*HSG(N)*TG(N)+ASX(N)*HXS(N)+  
2      TX1(N))-T1*TS2(N)
000031      S1(N)=-T*SK(N)/DX/DX
000032      S2(N)=1.-2.*S1(N)*T1
000033      S3(N)=S1(N)
000034      10 CONTINUE
000035      S2(1)=S2(1)+S1(1)
000036      S1(1)=0.0
000037      S2(NDX1)=S2(NDX1)+S3(NDX1)
000038      S3(NDX1)=0.
000039      NSG=NDXM+1
000040      S2(NDXM)=S2(NDXM)+S3(NDXM)
000041      S3(NDXM)=0.
000042      S2(NSG)=S2(NSG)+S1(NSG)
000043      S1(NSG)=0.0
000044      CALL FDEQIM(S1,S2,S3,B1,TS,NDX1)
000045      RETURN
000046      END

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* ELT TSORBA, 1, 710719, 62352 + 1

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000001      SUBROUTINE TSORBA
000002      COMMON/AD/ TG(20),PH20I ,TGI ,PA ,      PK (2,20),PC02I ,TS (20) *NEW
000003      1,TC (20),TX (20),TS1 (20),TS2 (20),TX1 (20),TX2 (20),TC1 (20), *NEW
000004      2TC2 (20),W (4,20),PT (20),      GMR ,GMW,GVIS, PN2,P02, *NEW
000005      3      ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20), *NEW
000006      4AVX(20),RHOG(20),RHOS(20),RHOS(20),RHOC(20),RHOX(20), *NEW
000007      5CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20), *NEW
000008      6POUT(10),TIMET(10),WTACMS,WTSG ,PUMP(10),VPUMP(10),CPP(20), *NEW
000009      7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20), *NEW
000010      8      HXG(20),HXS(20),HXC(20),HSG(20), *NEW
000011      9SK(20),TKX(20),DH(20),DIF(20),CK(20),UC(20),T268,TOTCO2,TOTH20, *NEW
000012      1SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX, *NEW
000013      1 TOTKWH,HTR(20),WC,TOTHTC,WCC,PC02A,VC02A,SABC02, TC02A, *NEW
000014      1RS1(20,9),      A(20),F(20),C(20),VS(20),DVS(20),DVS1(20),RS(20), *NEW
000015      1UG(20),FS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20), *NEW
000016      2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20), *NEW
000017      3FR(2,20),      P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3 *NEW
000018      4(20,4),      C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20), *NEW
000019      5      WM(2),TIME,CYCLE,DTO,      DTMAX,WI,TI,PC02C, *NEW
000020      6VOLCAR,RC02C, *NEW
000021      7NCYCLT,NPRINT,NCYCLE,NDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SABC05 *NEW
000022      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B, *NEW
000023      1      CP1,CP2,X,      C1P,C2P,C3P,D1P *NEW
000024      DIMENSION S1(41),S2(41),S3(41),B1(41) *NEW
000025      DO 10 N=1,NDX1 *NEW
000026      T=(DT+DTO)/CPS(N)/RHOSB(N) *NEW
000027      T1=0.5*T*(ASG(N)*HSG(N)+ASX(N)*HXS(N)) *NEW
000028      CS1(N)=CS1(N)*(1.0+T1) *NEW
000029      CS2(N)=CS2(N)*(1.0+T1) *NEW
000030      I=IFN(N,NDXM) *NEW
000031      TGAVG1=TG(N) *NEW
000032      B1(N) =TS2(N)+CS1(N)* *NEW
000033      1PK(I,N). *NEW
000034      2      -CS2(N)*(P1(N)+P2(N))*(W(NDR4,N)-WS(N))+ *NEW
000035      1P3(N)* *NEW
000036      2PK(I,N) *NEW
000037      3      )+T*(ASG(N)*HSG(N)*TGAVG1+ *NEW
000038      4ASX(N)*HXS(N)*TX1(N))-T1*TS2(N) *NEW
000039      S1(N)=-T*SK(N)/DX/DX *NEW
000040      S2(N)=1.-2.*S1(N)+T1 *NEW
000041      S3(N)=S1(N) *NEW
000042      10 CONTINUE *NEW
000043      S2(1)=S2(1)+S1(1) *NEW
000044      S1(1)=0.0 *NEW
000045      S2(NDX1)=S2(NDX1)+S3(NDX1) *NEW
000046      S3(NDX1)=0. *NEW
000047      NSG=NDXM+1 *NEW
000048      S2(NDXM)=S2(NDXM)+S3(NDXM) *NEW
000049      S3(NDXM)=0. *NEW
000050      S2(NSG)= S2(NSG)+S1(NSG) *NEW
000051      S1(NSG)=0.0 *NEW
000052      CALL FDEQIM(S1,S2,S3,B1,TS,NDX1) *NEW
000053      RETURN *NEW
000054      END *NEW

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@ ELT XYZMAP,1,710514, 38520 , 1

```

J00001      FUNCTION XYZMAP(IND,X,Y,NP,Z,NC,IDX,IDY,BX,BY,ANS)
J00002      C
J00003      C      FUNCTION XYZMAP HAS THE CAPABILITY OF SUBROUTINES MAPRDY + LAGIN2.
J00004      C      ANSWER IS ALSO AVAILABLE AT LOCATION (ANS).
J00005      C      ALSO CAPABLE OF HANDLING MAP THAT HAS Z-LINES CROSSING EACH OTHER.
J00006      C
J00007      C      X=ABSCISSA, Y=ORDINATE, Z=THIRD PARAMETER.
J00008      C
J00009      C      IND=0, Z=F(X,Y), (EQUIVALENT TO SUBROUTINE MAPRDY).
J00010      C      IND=1, Y=F(X,Z), (EQUIVALENT TO SUBROUTINE MAPRDY),
J00011      C      IND=-1, Y=F(X) ONLY, (EQUIVALENT TO LAGIN2), THEN Z,NC,IDX, AND AY
J00012      C      ARE DUMMY VARIABLES THAT ARE NOT NEEDED IN ACTUAL INTERPOLATION.
J00013      C
J00014      C      XS MUST BE STORED IN ASCENDING ORDER FOR EACH Z, SIMILARLY,
J00015      C      SMALLEST Z BE FED IN AS Z(1), ZS ARE IN ASCENDING ORDER.
J00016      C      XS NEED NOT BE THE SAME VALUES FOR VARIOUS ZS.
J00017      C      X,Y AND Z ARE TO BE DIMENSIONED IN THE MAIN (OR CALLING) PROGRAM,
J00018      C      THEY MUST BE DIMENSIONED NOT LESS THAN *** X(NP*NC), Y(NP*NC) AND
J00019      C      Z(NC) *** NOTE NC MAY NOT BE GREATER THAN 20 ***
J00020      C
J00021      C      NP=NUMBER OF POINTS PER CURVE (OR NUMBER OF X,Y PAIRS FOR EACH Z).
J00022      C      NC=NUMBER OF CURVES (OR NUMBER OF ZS), 1 TO A MAXIMUM OF 20
J00023      C
J00024      C      IDX=POINTS USED FOR INTERPOLATION IN X-DIRECTION,
J00025      C      IDY=POINTS USED FOR INTERPOLATION IN Y-DIRECTION (IND=0),
J00026      C      OR IN Z-DIRECTION (IND=1).
J00027      C      IDX OR IDY CAN EITHER BE 2 OR 3 ONLY.
J00028      C      BX=FIRST INDEPENDENT VARIABLE.
J00029      C      BY=SECOND INDEPENDENT VARIABLE, (WHEN IND=0 OR 1 ONLY).
J00030      C      BY=Y INDEPENDENT VARIABLE, WHEN (IND=0).
J00031      C      BY=Z INDEPENDENT VARIABLE, WHEN (IND=1).
J00032      C      ANS=DEPENDENT VARIABLE Z(X=AX,Y=Ay), WHEN IND=0,
J00033      C      ANS=DEPENDENT VARIABLE Y(X=AX,Z=Ay), WHEN IND=1,
J00034      C      ANS=DEPENDENT VARIABLE Y(X=AX), WHEN IND=-1.
J00035      C
J00036      C      NO PRINT OUT, IF DATA OFF THE RANGE OF MAP OR CURVE,
J00037      C      THEN, USE 2-POINT INTERPOLATIONS AUTOMATICALLY.
J00038      C
J00039      C      *****
J00040      C      XS, YS, AND ZS ARE READ IN IN MAIN PROGRAM RECOMMENDED AS FOLLOWS,
J00041      C      C4100 FORMAT(8I10)      *****
J00042      C      C4101 FORMAT(8F10.0)      *****
J00043      C      ***** FOR IND=0 OR 1 *****
J00044      C      C4101 READ (5,4100)      NP,NC      *****
J00045      C      DO 100 N=1,NC      *****
J00046      C      READ (5,4101)      Z(N)      *****
J00047      C      ME=N*NP      *****
J00048      C      MS=ME-NP+1      *****
J00049      C      100 READ (5,4101)      (X(M),Y(M),M=MS,ME)      *****
J00050      C      ***** FOR IND=-1 *****
J00051      C      READ (5,4100)      NP      *****
J00052      C      READ (5,4101)      (X(M),Y(M),M=1,np)      *****
J00053      C      *****
J00054      C      DIMENSION X(2),Y(2),Z(2),ZZ(20),ZX(20)
J00055      C
J00056      C      JS=1
J00057      C      IF (IND) 105,106,103
J00058      C      103 DO 104 I=1,NC

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000059      104 ZX(I)=Z(1)
000060      GO TO 141
000061      105 JE=1
000062      GO TO 108
000063      106 DO 107 I=1,NC
000064      107 ZZ(I)=Z(I)
000065      JE=NC
000066      NCROSS=0
000067      108 DO 126 J=JS,JE
000068      JX2=(J-1)*NP
000069      DO 109 I=1,NP
000070      J2=I+JX2
000071      IF (BX-X(J2)) 114,110,109
000072      109 CONTINUE
000073      GO TO 119
000074      110 ANS=Y(J2)
000075      GO TO 123
000076      114 IF(I-IDX)120,120,119
000077      119 JX2=J2-IDX
000078      120 IS=JX2+1
000079      IE=JX2+IDX
000080      IF(IDX.GT.2) GO TO 122
000081      121 ANS=(Y(IE)*(BX-X(IS))-Y(IS)*(BX-X(IE)))/(X(IE)-X(IS))
000082      GO TO 123
000083      122 IM=IS+1
000084      G1=(BX-X(IS))/(X(IM)-X(IE))
000085      G2=(BX-X(IM))/(X(IE)-X(IS))
000086      G3=(BX-X(IE))/(X(IS)-X(IM))
000087      ANS=-Y(IS)*G2*G3-G1*(Y(IM)*G3+Y(IE)*G2)
000088      123 IF (IND) 158,125,124
000089      124 Z(J)=ANS
000090      GO TO 126
000091      125 ZX(J)=ANS
000092      IF(ANS.LT.ZX(1)) NCROSS=1
000093      126 CONTINUE
000094      IF(IND.NE.0) GO TO 1151
000095      IF(NCROSS.EQ.0) GO TO 141
000096
000097      C      DO 130 K=2,NC
000098      JMIN=K-1
000099      DO 129 IP=K,NC
000100      IF (ZX(IP)-ZX(JMIN)) 128,128,129
000101      128 JMIN=IP
000102      129 CONTINUE
000103      IK=K-1
000104      C1=ZX(JMIN)
000105      Z1=ZZ(JMIN)
000106      ZX(JMIN)=ZX(IK)
000107      ZZ(JMIN)=ZZ(IK)
000108      ZX(IK)=C1
000109      130 ZZ(IK)=Z1
000110      C
000111      141 ICPY= IDY-1
000112      DO 142 I=1,NC
000113      IF(BY-ZX(I))145,144,142
000114      142 CONTINUE
000115      JS=NC-ICPY
000116      GO TO 147
000117      144 JS=I
000118      IF (IND.EQ.0) GO TO 151

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000119      JE=JS
000120      GO TO 108
000121      145 IF(I.LE.IDY) GO TO 147
000122      146 JS=I-ICPY
000123      147 JE=JS+ICPY
000124      IF (IND) 108,1152,108
000125      C Y=F(X,Z) OR Z=F(X,Y) CALCULATION DEPENDING ON IND=0 OR 1.
000126      151 ANS=ZZ(JS)
000127      GO TO 158
000128      1151 IF(JE.EQ.JS) GO TO 151
000129      1152 IF(IDY.GT.2) GO TO 153
000130      152 ANS=(ZZ(JE)*(BY-ZX(JS))-ZZ(JS)*(BY-ZX(JE)))/(ZX(JE)-ZX(JS))
000131      GO TO 158
000132      153 JM=JS+1
000133      G1=(BY-ZX(JS))/(ZX(JM)-ZX(JE))
000134      G2=(BY-ZX(JM))/(ZX(JE)-ZX(JS))
000135      G3=(BY-ZX(JE))/(ZX(JS)-ZX(JM))
000136      ANS=-ZZ(JS)*G2*G3=G1*(ZZ(JM)*G3+ZZ(JE)*G2)
000137      158 XYZMAP=ANS
000138      RETURN
000139      END

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